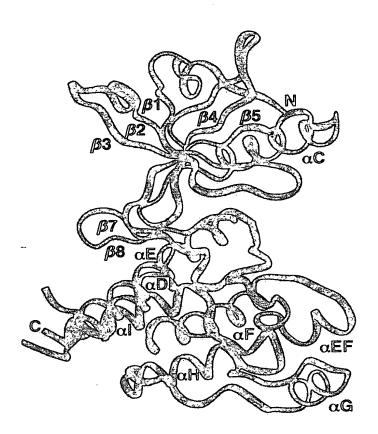
FIG. 1a

	1/67		**
863 509 1025 856 622	923 568 1083 916 681	953 586 1095 946 741	1010 605 1114 1004 800
nucleotide-binding loop VEGF-R2 806 MDPDELPLDEHCERLPYDASKWEFPRDRLKLGK PLGRGAFGQVE ADAFGIDKTATCR FGFR1 456MLAGVSEYELP-EDPRWELPRDRLVLGK PLGEGCFGQVL AEA I GLDKDKPNRVT I RK 978VFPCSVYVPDEWEVSREKITLL RELGOGSFGMVEGNARDI I KGEAET VEGF-R1 799 MDPDEVPLDEQCERLPYDASKWEFARERLKLGK SLGRGAFGKVGA SAFGIKKSPTCR PDGFRα 576DPMQLPYD-SRWEFPRDGLVLGR VLGSGAFGKVEGTAYGLSRSQPVM	VEGF-R2 864 TVAVKMLKEGATHSEHRALMSELKILIHIGHHLNVVNLLGACTKPGGPLMVIVEFCKFGN FGFR1 510 KVAVKMLKSDATEKDLSDLISEMEMMKMIGKHKNIINLLGACT-QDGPLYVIVEYASKGN IRK 1026 RVAVKTVNESASLRERIEFLNEASVMKGFTCH-HVVRLLGVVSK-GQPTLVVMELMAHGD VEGF-R1 857 TVAVKMLKEGATASEYKALMTELKILTHIGHHLNVVNLLGACTKOGGPLMVIVEYCKYGN PDGFRα 623 KVAVKMLKFTARSSEKQALMSELKIMTHLGPHLNIVNLLGACTK-SGPIYIITEYCFYGD	VEGF-R2 924 LSTYLRSKRNEFVPYKTKGARFRQGKDYVG	VEGF-R2 954AIPVDLKRRLDSITSSQSSASSGFVEEKSLSDVEEEEAPEDLYKDFLTLEHLICYSF FGFR1 587

FIG. 1b

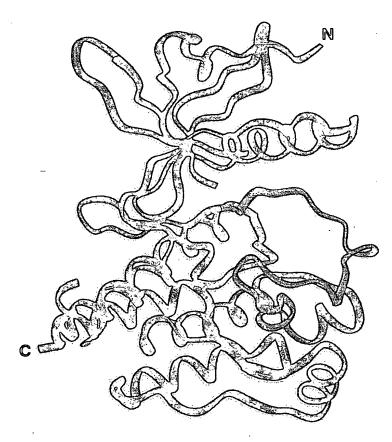
	2/67					
	1070 665 1174 1064 860	923 568 1083 916 681	1171 765 1274 1165 961			
catalytic loop 87 B8 activation loop	VEGF-R2 1011 QVAKGMEFDLASRKCIHRDLAARNILLSEKNVVKICDFGLARDIYKDPDYVRKGDARLPLK FGFR1 606 QVARGMEYSLASKKCIHRDLAARNVLVTEDNVMKIADFGLARDIHHIDYYKKTTNGRLPVK IRK 1115 EIADGMEY-LNAKKFVHRDLAARNCMVAHDFTVKIGDFGMTRDIYETDYYRKGGKGLLPVR VEGF-R1 1005 QVARGMEFDLSSRKCIHRDLAARNILLSENNVVKIDDFGLARDIYKNPDYVRKGDTRLPLK PDGFRα 801 QVARGMEF-LASKKCIHRDLAARNVLLAQGKIVKIDDFGLARDIMHDSNYVSKGSTFLPVK	VEGF - R2 1071 WMAPETIFDRYYTIQSDVWSFGVLLWEIFSLGASPYPGVKIDEEFCRRLKEGTRMRRAPDY FGFR1 666 WMAPEALFDRIYTHQSDVWSFGVLLWEIFTLGGSPYPGVPELF - KLLKEGHRMDRKPSN ITAS WMAPESLKDGVFTTSSDMWSFGVV WEITSLAEQPYQGLSNEQVL - KFVMDGGYLDLQPDN VEGF - R1 1065 WMAPESIFDKIYSTKSDVWSYGVLLWEIFSLGGSPYPGVQMDEDFCSRLREGMRMRRAPEY PDGFRα 861 WMAPESIFDNLYTTLSDVWSYGILLWEIFSLGGTPYPGMMVDSTFYNKIKSGYRMAFKPDH	VEGF-R2 1131 TTPEMYQTMLDCWHGEPSQRPTFSELVEHLGNLLQANAQQD FGFR1 725 CTNELYMMMRDCWHAVPSQRPTFKQLVEDLDRIVALTSNQE IRK 1234 CPERVTDLMRMCWQFNPNMRPTFLEIVNLLKDDLHPSFPEV VEGF-R1 1125 STPEIYQIMLDCWHRDPKERPRFAELVEKLGDLLQANVQQD PDGFRα 921 ATSEVYEIMVKCWNSEPEKRPSFYHLSEIVENLLPGQYKKS			

FIG. 2a



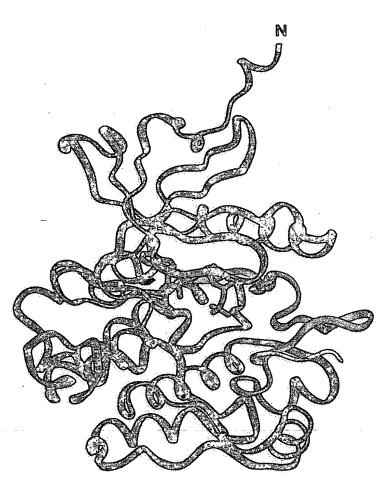
VEGFR2D50P

FIG. 2b

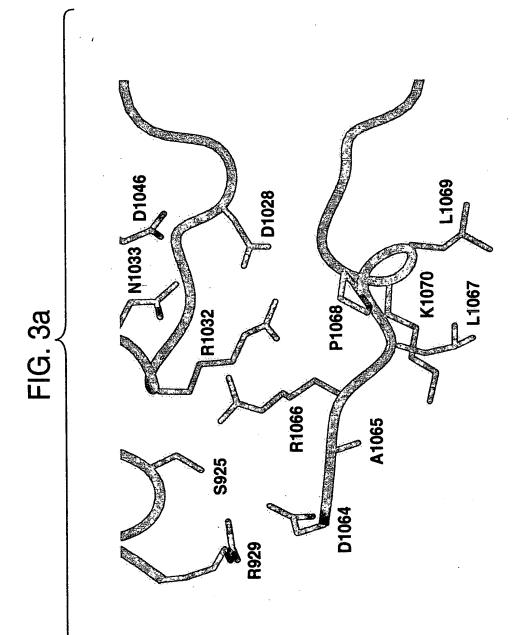


FGFR1

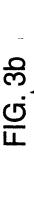
FIG. 2c



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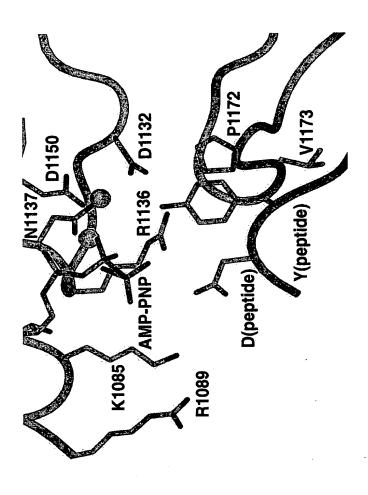
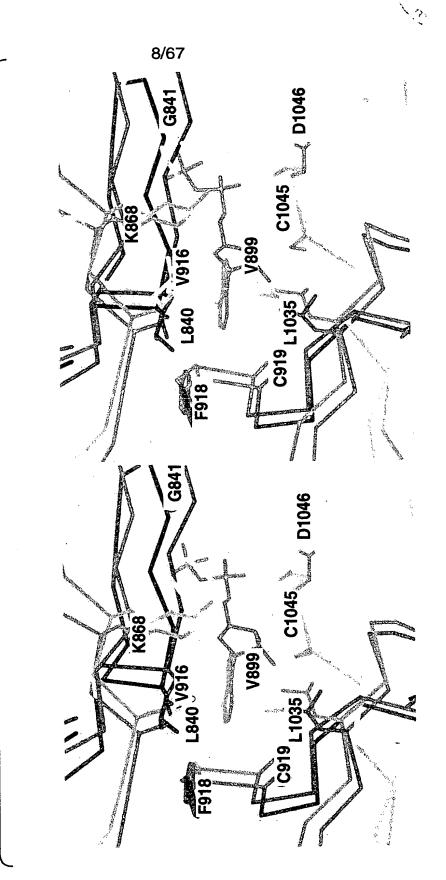


FIG. 4



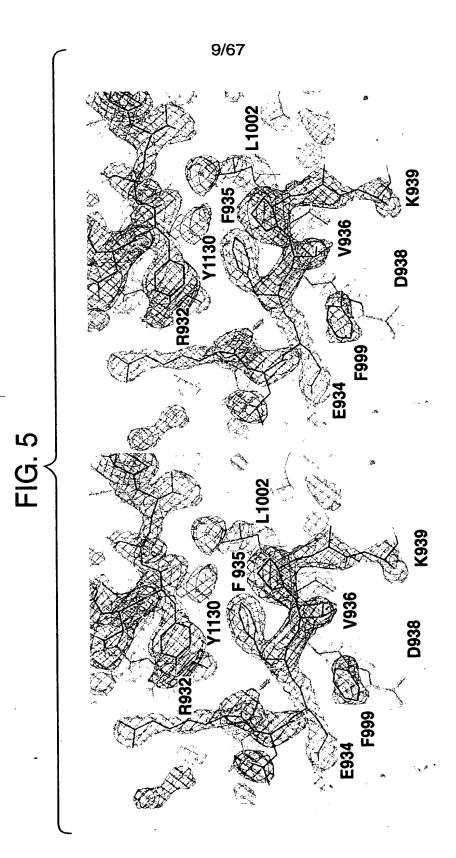


FIG. 6

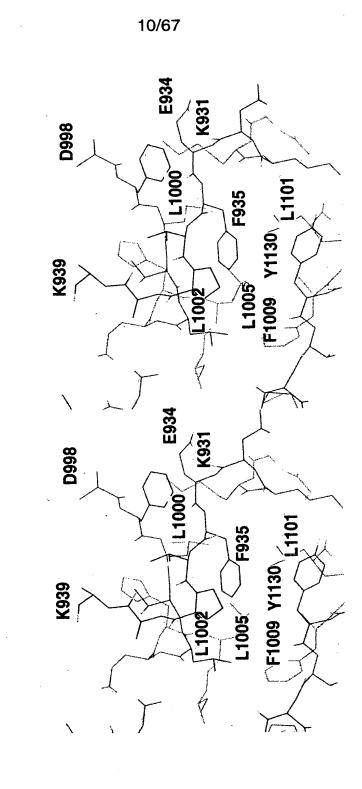


FIG. 7(1)

ATOM 1 CB LEU 820 49.908 45.905 17.938 1.00 48.95 **ATOM** 2 CG LEU 820 50.568 45.069 16.833 1.00 43.57 ATOM 3 CD1 LEU 820 50.004 45.358 15.456 1.00 43.59 4 CD2 LEU 820 **ATOM** 52.066 45.345 16.886 1.00 47.45 ATOM 5 C LEU 820 49.216 48.321 17.530 1.00 48.14 6 O LEU 820 48.196 48.587 18.187 1.00 52.58 ATOM **ATOM** 9 N LEU 820 50.481 47.725 19.581 1.00 53.68 11 CA LEU 820 50.302 47.387 18.117 1.00 50.63 **ATOM** 12 N PRO 821 49.435 48.842 16.306 1.00 41.32 **ATOM ATOM** 13 CD PRO 821 50.680 48.870 15.520 1.00 45.54 14 CA PRO 821 48.465 49.733 15.700 1.00 31.06 **ATOM** 49.067 49.985 14.352 1.00 28.89 **ATOM** 15 CB PRO 821 16 CG PRO 821 50.509 50.148 14.734 1.00 43.44 ATOM ATOM 17 C PRO 821 47.123 49.165 15.569 1.00 26.14 18 O PRO 821 46.948 47.970 15.374 1.00 26.03 ATOM ATOM 19 N TYR 822 46.154 50.024 15.776 1.00 16.25 44.799 49.643 15.582 1.00 18.88 21 CA TYR 822 ATOM 22 CB TYR 822 44.061 49.519 16.916 1.00 17.42 **ATOM** ATOM 23 CG TYR 822 42.584 49.316 16.728 1.00 18.46 **ATOM** 24 CD1 TYR 822 41.674 50.341 17.047 1.00 21.12 25 CE1 TYR 822 40.314 50.206 16.812 1.00 13.80 **ATOM** 26 CD2 TYR 822 42.086 48.144 16.175 1.00 12.24 ATOM 27 CE2 TYR 822 40.714 47.997 15.951 1.00 13.44 ATOM 28 CZ TYR 822 39.838 49.028 16.268 1.00 14.38 **ATOM** 29 OH TYR 822 38.480 48.887 16.073 1.00 19.73 **ATOM ATOM** 31 C TYR 822 44.253 50.760 14.705 1.00 16.93 ATOM 32 O TYR 822 44.172 51.904 15.112 1.00 20.70 ATOM 33 N ASP 823 44.054 50.456 13.439 1.00 15.20 35 CA ASP 823 43.509 51.418 12.506 1.00 13.55 ATOM **ATOM** 36 CB ASP 823 43.856 50.945 11.091 1.00 11.37 ATOM 37 CG ASP 823 43.456 51.933 10.016 1.00 16.45 38 OD1 ASP 823 ATOM 42.546 52.754 10.258 1.00 21.86 ATOM 39 OD2 ASP 823 44.022 51.854 8.904 1.00 12.33 41.983 51.489 12.738 1.00 14.14 MOTA 40 C ASP 823 ATOM 41 O ASP 823 41.224 50.722 12.172 1.00 19.73 42 N ALA 824 41.539 52.415 13.572 1.00 11.88 ATOM 44 CA ALA 824 40.126 52.554 13.876 1.00 14.80 MOTA ATOM 45 CB ALA 824 39.928 53.610 14.973 1.00 12.02 39.259 52.893 12.658 1.00 19.09 MOTA 46 C ALA 824 47 O ALA 824 38.062 52.610 12.641 1.00 23.54 MOTA

FIG. 7(2)

39.857 53.496 11.635 1.00 18.25 ATOM 48 N SER 825 39.118 53.867 10.450 1.00 12.65 ATOM 50 CA SER 825 40.023 54.678 9.543 1.00 11.88 ATOM 51 CB SER 825 52 OG SER 825 39.315 55.003 8.370 1.00 20.94 ATOM 38.669 52.594 9.746 1.00 12.30 **ATOM** 54 C SER 825 37.543 52.461 9.317 1.00 14.94 55 O SER 825 **ATOM** 56 N LYS 826 39.557 51.633 9.642 1.00 14.98 ATOM 39.188 50.396 8.988 1.00 22.45 58 CA LYS 826 ATOM 40.445 49.660 8.483 1.00 16.46 59 CB LYS 826 ATOM ATOM 60 CG LYS 826 40.091 48.370 7.820 1.00 23.00 6.657 1.00 26.19 61 CD LYS 826 40.962 48.071 ATOM 7.092 1.00 35.70 62 CE LYS 826 42.391 48.041 ATOM 43.272 48.003 5.891 1.00 40.17 ATOM 63 NZ LYS 826 67 C LYS 826 38.324 49.437 9.839 1.00 21.47 ATOM 37.363 48.850 9.336 1.00 22.56 68 O LYS 826 ATOM 69 N TRP 827 38.589 49.376 11.144 1.00 20.96 ATOM 37.917 48.406 11.996 1.00 16.87 71 CA TRP 827 ATOM 72 CB TRP 827 38.974 47.620 12.785 1.00 18.53 ATOM 39.942 46.898 11.910 1.00 12.95 ATOM 73 CG TRP 827 39.643 45.810 11.029 1.00 9.73 ATOM 74 CD2 TRP 827 75 CE2 TRP 827 40.795 45.562 10.274 1.00 9.36 MOTA 38.505 45.038 10.801 1.00 11.54 76 CE3 TRP 827 MOTA 41.233 47.231 11.684 1.00 12.87 77 CD1 TRP 827 ATOM **ATOM** 78 NEI TRP 827 41.753 46.440 10.689 1.00 10.49 40.848 44.565 9.299 1.00 12.36 ATOM 80 CZ2 TRP 827 38.556 44.053 9.826 1.00 10.55 ATOM 81 CZ3 TRP 827 39.718 43.830 9.087 1.00 11.88 MOTA 82 CH2 TRP 827 36.830 48.795 12.953 1.00 17.75 MOTA 83 C TRP 827 84 O TRP 827 35.985 47.951 13.271 1.00 15.08 ATOM ATOM 85 N GLU 828 36.855 50.043 13.416 1.00 16.92 35.908 50.518 14.413 1.00 19.52 87 CA GLU 828 MOTA 88 CB GLU 828 36.289 51.920 14.885 1.00 17.10 ATOM 35.581 52.363 16.148 1.00 12.70 ATOM 89 CG GLU 828 36.106 51.707 17.400 1.00 21.57 90 CD GLU 828 MOTA 37.219 51.118 17.386 1.00 21.15 MOTA 91 OE1 GLU 828 35.402 51.819 18.426 1.00 22.43 MOTA 92 OE2 GLU 828 93 C GLU 828 34.494 50.510 13.910 1.00 20.94 MOTA 34.245 51.024 12.818 1.00 26.92 GLU 828 MOTA 94 O 33.569 49.990 14.734 1.00 21.12 95 N PHE 829 ATOM 97 CA PHE 32.138 49.880 14.391 1.00 17.93 ATOM 829 31.791 48.400 14.160 1.00 16.42 ATOM 98 CB PHE 829 30.384 48.164 13.669 1.00 20.17 MOTA 99 CG PHE 829

FIG. 7(3)

30.020 48.484 12.363 1.00 21.31 100 CD1 PHE 829 **ATOM** 101 CD2 PHE 829 29.415 47.612 14.516 1.00 23.04 ATOM ATOM 102 CE1 PHE 829 28.712 48.254 11.921 1.00 18.76 28.093 47.375 14.071 1.00 15.20 **ATOM** 103 CE2 PHE 829 104 CZ PHE 829 27.750 47.692 12.792 1.00 17.17 **ATOM** 31.310 50.495 15.533 1.00 14.65 105 C PHE 829 **ATOM** 106 O PHE 829 31.574 50.211 16.686 1.00 16.15 **ATOM** 107 N PRO 830 30.270 51.298 15.224 1.00 13.29 **ATOM ATOM** 108 CD PRO 830 29.707 51.633 13.901 1.00 11.63 29.481 51.918 16.292 1.00 14.76 109 CA PRO 830 **ATOM** 110 CB PRO 830 28.636 52.948 15.565 1.00 13.82 **ATOM** 28.414 52.364 14.252 1.00 14.42 **ATOM** 111 CG PRO 830 28.629 51.005 17.098 1.00 19.79 **MOTA** 112 C PRO 830 113 O PRO 830 27.750 50.339 16.562 1.00 26.60 ATOM 114 N ARG 831 28.830 51.060 18.410 1.00 18.39 **ATOM** 28.085 50.246 19.335 1.00 14.56 116 CA ARG 831 **ATOM ATOM** 117 CB ARG 831 28.469 50.580 20.743 1.00 11.53 29.808 50.050 21.092 1.00 12.65 118 CG ARG 831 **ATOM** 30.117 50.265 22.554 1.00 12.46 ATOM 119 CD ARG 831 31.261 51.148 22.584 1.00 20.55 **ATOM** 120 NE ARG 831 32.469 50.756 22.885 1.00 12.04 **ATOM** 122 CZ ARG 831 32.688 49.518 23.234 1.00 23.80 123 NH1 ARG 831 **ATOM** 33.467 51.501 22.526 1.00 23.84 **ATOM** 126 NH2 ARG 831 26.625 50.415 19.174 1.00 18.55 **ATOM** 129 C ARG 831 25.852 49.561 19.607 1.00 25.61 **ATOM** 130 O ARG 831 131 N ASP 832 26.221 51.517 18.552 1.00 25.32 **ATOM** 24.794 51.734 18.354 1.00 29.47 133 CA ASP 832 **ATOM** ATOM 134 CB ASP 832 24.393 53.230 18.408 1.00 34.15 24.817 54.036 17.174 1.00 33.50 135 CG ASP 832 **ATOM** 25.519 53.528 16.280 1.00 34.09 136 OD1 ASP 832 ATOM ATOM 137 OD2 ASP 832 24.422 55.216 17.110 1.00 41.48 24.230 51.000 17.139 1.00 27.13 138 C ASP 832 ATOM 23.023 50.905 16.991 1.00 28.08 **ATOM** 139 O ASP 832 140 N ARG 833 25.104 50.466 16.290 1.00 24.18 ATOM 24.684 49.695 15.134 1.00 19.93 142 CA ARG 833 ATOM 143 CB ARG 833 25.661 49.902 14.011 1.00 25.94 ATOM 25.313 51.073 13.158 1.00 38.97 144 CG ARG 833 MOTA 25.929 50.901 11.766 1.00 53.19 ATOM 145 CD ARG 833 MOTA 146 NE ARG 833 25.525 51.930 10.807 1.00 63.47 25.419 53.229 11.087 1.00 70.42 MOTA 148 CZ ARG 833 25.040 54.080 10.139 1.00 74.08 149 NH1 ARG 833 ATOM 25.695 53.690 12.306 1.00 72.08 MOTA 152 NH2 ARG 833 24.656 48.218 15.498 1.00 18.62 155 C ARG 833 MOTA

FIG. 7(4)

156 O ARG 833 24.289 47.370 14.690 1.00 18.27 **ATOM** ATOM 157 N LEU 834 25.013 47.943 16.747 1.00 18.35 159 CA LEU 834 25.089 46.600 17.329 1.00 22.59 **ATOM** 160 CB LEU 834 26.488 46.398 17.946 1.00 25.91 **ATOM** 27.073 45.003 18.139 1.00 24.64 **ATOM** 161 CG LEU 834 162 CD1 LEU 834 27.185 44.327 16.805 1.00 21.77 **ATOM** 28.428 45.085 18.785 1.00 17.43 **ATOM** 163 CD2 LEU 834 ATOM 164 C LEU 834 23.988 46.326 18.387 1.00 24.77 23.886 46.973 19.433 1.00 24.03 **MOTA** 165 O LEU 834 23.173 45.335 18.087 1.00 28.94 166 N LYS 835 ATOM 168 CA LYS 835 22.072 44.942 18.940 1.00 32.84 **ATOM** 20.794 44.913 18.081 1.00 31.34 169 CB LYS 835 **ATOM** 19.529 44.697 18.839 1.00 36.63 170 CG LYS 835 **ATOM** 171 CD LYS 835 18.359 44.407 17.940 1.00 39.31 **ATOM** 17.074 44.414 18.783 1.00 48.99 172 CE LYS 835 ATOM 173 NZ LYS 835 17.074 43.448 19.950 1.00 48.86 **ATOM** 22.431 43.532 19.420 1.00 31.79 177 C LYS 835 **ATOM** 22.408 42.609 18.616 1.00 34.57 178 O LYS 835 **ATOM ATOM** 179 N LEU 836 22.854 43.395 20.680 1.00 33.17 181 CA LEU 836 23.229 42.101 21.277 1.00 34.01 ATOM 23.970 42.292 22.593 1.00 33.96 **ATOM** 182 CB LEU 836 25.400 42.796 22.462 1.00 42.50 ATOM 183 CG LEU 836 26.082 42.858 23.854 1.00 41.15 **ATOM** 184 CD1 LEU 836 26.153 41.860 21.501 1.00 40.93 **ATOM** 185 CD2 LEU 836 22.053 41.181 21.547 1.00 33.27 ATOM 186 C LEU 836 21.017 41.631 22.025 1.00 31.15 **ATOM** 187 O LEU 836 22.268 39.882 21.330 1.00 36.34 **ATOM** 188 N GLY 837 21.228 38.881 21.536 1.00 34.95 190 CA GLY 837 MOTA 21.603 37.761 22.497 1.00 35.64 191 C GLY 837 **ATOM** 22.203 37.980 23.554 1.00 39.23 ATOM 192 O GLY 837 21.254 36.541 22.126 1.00 35.31 193 N LYS 838 ATOM 195 CA LYS 838 21.531 35.375 22.962 1.00 37.86 ATOM 196 CB LYS 838 20.647 34.192 22.539 1.00 41.52 MOTA 22.991 34.935 22.989 1.00 35.93 197 C LYS 838 MOTA 23.650 34.851 21.946 1.00 34.37 198 O LYS 838 ATOM 23.499 34.608 24.187 1.00 33.68 199 N PRO 839 ATOM 22.820 34.757 25.486 1.00 34.48 200 CD PRO 839 MOTA 24.880 34.158 24.363 1.00 37.11 ATOM 201 CA PRO 839 24.927 33.750 25.833 1.00 37.46 202 CB PRO 839 **ATOM** 23.970 34.710 26.472 1.00 37.04 **ATOM** 203 CG PRO 839 25.148 32.963 23.474 1.00 39.09 24.303 32.085 23.327 1.00 38.13 204 C PRO 839 ATOM ATOM 205 O PRO 839 26.261 33.013 22.767 1.00 43.08 206 N LEU 840 ATOM

FIG. 7(5)

26.646 31.915 21.917 1.00 47.73 ATOM 208 CA LEU 840 27.396 32.426 20.692 1.00 41.83 ATOM 209 CB LEU 840 26.386 32.957 19.697 1.00 39.60 ATOM 210 CG LEU 840 27.080 33.697 18.595 1.00 42.69 **ATOM** 211 CD1 LEU 840 25.582 31.795 19.156 1.00 38.40 212 CD2 LEU 840 **ATOM** 27.523 30.987 22.747 1.00 54.84 **ATOM** 213 C LEU 840 214 O LEU 840 27.479 29.768 22.577 1.00 59.76 **ATOM** 28.248 31.563 23.706 1.00 60.51 215 N GLY 841 **ATOM** 217 CA GLY 841 29.140 30.781 24.547 1.00 60.96 ATOM 29.660 31.544 25.750 1.00 63.95 218 C GLY 841 ATOM 29.497 32.764 25.857 1.00 64.35 219 O GLY 841 ATOM 30.279 30.809 26.668 1.00 65.26 **ATOM** 220 N ARG 842 30.823 31.388 27.887 1.00 65.12 ATOM 222 CA ARG 842 30.027 30.897 29.091 1.00 61.50 223 CB ARG 842 ATOM 32.300 30.995 28.004 1.00 64.23 224 C ARG 842 ATOM 32.957 30.720 26.986 1.00 68.80 **ATOM** 225 O ARG 842 32.822 31.003 29.226 1.00 60.14 226 N GLY 843 ATOM **ATOM** 228 CA GLY 843 34.206 30.639 29.453 1.00 60.53 229 C GLY 843 34.676 31.165 30.789 1.00 62.56 **ATOM** 33.902 31.764-31.535 1.00 61.31 230 O GLY 843 ATOM ATOM 231 N ALA 844 35.925 30.888 31.140 1.00 66.30 36.450 31.390 32.403 1.00 69.69 233 CA ALA 844 MOTA 37.655 30.574 32.851 1.00 68.47 234 CB ALA 844 **ATOM** 36.839 32.855 32.212 1.00 73.15 MOTA 235 C ALA 844 36.723 33.667 33.144 1.00 75.00 **ATOM** 236 O ALA 844 237 N PHE 845 37.251 33.184 30.981 1.00 76.12 ATOM 37.699 34.538 30.618 1.00 74.99 **ATOM** 239 CA PHE 845 240 CB PHE 845 39.135 34.479 30.014 1.00 72.01 **ATOM MOTA** 241 C PHE 845 36.766 35.353 29.700 1.00 73.81 36.404 36.499 30.020 1.00 76.82 242 O PHE 845 ATOM 36.368 34.767 28.576 1.00 68.48 243 N GLY 846 ATOM 35.527 35.495 27.645 1.00 61.76 ATOM 245 CA GLY 846 34.102 35.023 27.606 1.00 57.98 246 C GLY 846 MOTA 247 O GLY 846 33.658 34.305 28.491 1.00 59.43 MOTA 248 N GLN 847 33.400 35.413 26.553 1.00 55.08 MOTA 32.006 35.050 26.354 1.00 52.26 250 CA GLN 847 MOTA 31.160 35.668 27.449 1.00 55.14 251 CB GLN 847 MOTA 29.706 35.703 27.075 1.00 61.40 252 CG GLN 847 MOTA 28.951 36.735 27.844 1.00 65.75 253 CD GLN 847 MOTA 254 OE1 GLN 847 27.772 36.543 28.150 1.00 69.74 ATOM 29.614 37.852 28.166 1.00 68.83 255 NE2 GLN 847 MOTA 31.508 35.573 25.001 1.00 47.29 MOTA 258 C GLN 847 31.637 36.764 24.713 1.00 52.89 259 O GLN 847 ATOM

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FIG. 7(6)

30.912 34.707 24.195 1.00 38.17 **ATOM** 260 N VAL 848 30.418 35.122 22.898 1.00 30.28 262 CA VAL 848 **ATOM** 30.792 34.137 21.833 1.00 28.01 263 CB VAL 848 **ATOM** 30.542 34.744 20.442 1.00 23.32 264 CG1 VAL 848 ATOM 32.239 33.759 22.016 1.00 22.18 **ATOM** 265 CG2 VAL 848 28.920 35.262 22.939 1.00 31.80 266 C VAL 848 **ATOM** 28.221 34.525 23.625 1.00 32.87 ATOM 267 O VAL 848 28.410 36.196 22.166 1.00 29.87 268 N ILE 849 ATOM 270 CA ILE 849 26.990 36.436 22.159 1.00 25.35 ATOM 26.602 37.448 23.328 1.00 31.46 **ATOM** 271 CB ILE 849 27.766 38.373 23.732 1.00 32.09 **ATOM** 272 CG2 ILE 849 273 CG1 ILE 849 25.353 38.244 23.003 1.00 31.00 **ATOM** 24.895 39.035 24.199 1.00 37.56 274 CD1 ILE 849 ATOM 275 C ILE 849 26.493 36.851 20.798 1.00 23.02 **ATOM** 276 O ILE 849 27.167 37.540 20.070 1.00 27.56 **ATOM** 25.376 36.294 20.390 1.00 25.56 277 N GLU 850 **ATOM** 24.802 36.626 19.107 1.00 26.63 279 CA GLU 850 MOTA 23.577 35.785 18.894 1.00 27.45 **ATOM** 280 CB GLU 850 281 CG GLU 850 23.414 35.361 17.487 1.00 34.57 ATOM 22.155 34.590 17.293 1.00 34.46 282 CD GLU 850 ATOM 21.602 34.655 16.184 1.00 42.38 ATOM 283 OE1 GLU 850 21.710 33.924 18.248 1.00 40.93 284 OE2 GLU 850 ATOM 285 C GLU 850 24.422 38.111 19.028 1.00 27.83 ATOM 24.240 38.755 20.047 1.00 25.02 ATOM 286 O GLU 850 24.291 38.640 17.814 1.00 29.11 ATOM 287 N ALA 851 23.958 40.043 17.621 1.00 27.32 289 CA ALA 851 ATOM 25.080 40.922 18.170 1.00 18.65 290 CB ALA 851 ATOM 23.731 40.387 16.160 1.00 26.61 291 C ALA 851 ATOM 24.328 39.785 15.283 1.00 26.99 MOTA 292 O ALA 851 22.836 41.343 15.917 1.00 30.82 293 N ASP 852 ATOM 22.538 41.862 14.566 1.00 31.76 ATOM 295 CA ASP 852 21.050 42.186 14.386 1.00 39.33 296 CB ASP 852 ATOM 20.222 40.993 13.993 1.00 47.41 297 CG ASP 852 ATOM 19.687 40.330 14.906 1.00 54.12 298 OD1 ASP 852 ATOM 20.066 40.754 12.775 1.00 53.02 299 OD2 ASP 852 ATOM 23.265 43.204 14.506 1.00 25.97 300 C ASP 852 ATOM 23.096 44.021 15.416 1.00 21.64 MOTA 301 O ASP 852 302 N ALA 853 24.099 43.411 13.495 1.00 20.18 MOTA 24.818 44.672 13.342 1.00 23.55 ATOM 304 CA ALA 853 305 CB ALA 853 26.305 44.440 13.292 1.00 23.32 MOTA 24.311 45.222 12.026 1.00 23.89 306 C ALA 853 ATOM 24.079 44.439 11.108 1.00 26.15 MOTA 307 O ALA 853 24.044 46.526 11.936 1.00 22.87 308 N PHE 854 ATOM

FIG. 7(7)

310 CA PHE 854 23.529 47.059 10.680 1.00 16.46 ATOM 22.487 48.135 10.901 1.00 23.71 ATOM 311 CB PHE 854 312 CG PHE 854 22.020 48.758 9.643 1.00 27.62 **ATOM** 22.476 50.011 9.266 1.00 28.26 **ATOM** 313 CD1 PHE 854 21.205 48.052 8.771 1.00 31.56 314 CD2 PHE 854 ATOM 22.136 50.549 8.025 1.00 30.16 315 CE1 PHE 854 **ATOM** 20.856 48.592 7.512 1.00 34.04 316 CE2 PHE 854 **ATOM** 21.328 49.838 7.145 1.00 28.32 317 CZ PHE 854 ATOM 24.618 47.569 9.794 1.00 14.10 ATOM 318 C PHE 854 25.493 48.299 10.209 1.00 17.34 319 O PHE 854 ATOM 320 N GLY 855 24.556 47.163 8.553 1.00 17.45 **ATOM** 25.559 47.571 7.604 1.00 18.50 ATOM 322 CA GLY 855 323 C GLY 855 26.988 47.318 8.020 1.00 22.65 **ATOM** 27.806 48.193 7.777 1.00 26.82 324 O GLY 855 ATOM 27.332 46.150 8.580 1.00 23.51 325 N ILE 856 **ATOM** 28.740 45.886 8.983 1.00 24.11 327 CA ILE 856 ATOM 328 CB ILE 856 28.868 44.692 9.980 1.00 27.72 MOTA 28.535 43.370 9.259 1.00 29.88 ATOM 329 CG2 ILE 856 30.282 44.663 10.608 1.00 23.26 **ATOM** 330 CG1 ILE 856 331 CD1 ILE 856 30.371 44.079 12.034 1.00 21.70 ATOM 29.704 45.665 7.805 1.00 24.83 MOTA 332 C ILE 856 7.950 1.00 28.37 30.918 45.721 ATOM 333 O ILE 856 29.145 45.460 6.626 1.00 27.69 **MOTA** 334 N ASP 857 29.926 45.248 5.420 1.00 31.23 336 CA ASP 857 **ATOM** 29.566 43.891 4.838 1.00 34.80 **ATOM** 337 CB ASP 857 ATOM 28.074 43.658 4.811 1.00 40.03 338 CG ASP 857 27.328 44.597 4.448 1.00 43.33 339 OD1 ASP 857 ATOM 340 OD2 ASP 857 27.641 42.549 5.200 1.00 46.87 **ATOM** 29.654 46.323 4.370 1.00 32.81 ATOM 341 C ASP 857 29.721 46.040 3.183 1.00 38.59 342 O ASP 857 ATOM 343 N LYS 858 29.299 47.529 4.813 1.00 34.74 ATOM 28.987 48.690 3.946 1.00 34.64 ATOM 345 CA LYS 858 MOTA 30.061 48.947 2.889 1.00 31.38 346 CB LYS 858 31.462 48.964 3.418 1.00 34.36 ATOM 347 CG LYS 858 31.605 49.890 4.603 1.00 39.41 MOTA 348 CD LYS 858 349 CE LYS 858 33.005 49.791 5.228 1.00 39.87 ATOM 34.059 50.089 4.218 1.00 39.89 350 NZ LYS 858 ATOM 27.629 48.709 3.254 1.00 32.27 **MOTA** 354 C LYS 858 355 O LYS 858 27.249 49.737 2.724 1:00 35.02 MOTA 26.891 47.607 3.258 1.00 32.20 356 N THR 859 MOTA 25.597 47.610 2.600 1.00 30.11 MOTA 358 CA THR 859 25.355 46.332 1.785 1.00 30.38 MOTA 359 CB THR 859 25.365 45.187 2.641 1.00 32.29 360 OG1 THR 859 ATOM

FIG. 7(8)

ATOM 362 CG2 THR 859 26.437 46.179 0.757 1.00 32.22 ATOM 24.450 47.839 3.546 1.00 28.71 363 C THR 859 24.577 47.647 4.750 1.00 30.55 ATOM 364 O THR 859 **ATOM** 365 N ALA 860 23.303 48.201 2.989 1.00 30.07 **ATOM** 367 CA ALA 860 22.123 48.474 3.784 1.00 28.01 ATOM 368 CB ALA 860 21.141 49.253 2.928 1.00 23.78 21.461 47.222 4.394 1.00 28.00 **ATOM** 369 C ALA 860 **ATOM** 370 O ALA 860 20.251 47.100 4.373 1.00 31.77 371 N THR 861 22.228 46.325 5.008 1.00 29.99 **ATOM** 373 CA THR 861 21.663 45.078 5.577 1.00 27.77 ATOM **ATOM** 374 CB THR 861 22.186 43.857 4.808 1.00 20.97 375 OG1 THR 861 23.614 43.926 4.687 1.00 27.23 **ATOM** 21.608 43.794 3.449 1.00 29.39 **MOTA** 377 CG2 THR 861 21.986 44.790 7.055 1.00 31.89 MOTA 378 C THR 861 379 O THR 861 23.095 45.077 7.532 1.00 34.73 **ATOM** 380 N CYS 862 21.037 44.183 7.770 1.00 34.09 ATOM 21.250 43.805 9.178 1.00 31.63 ATOM 382 CA CYS 862 383 CB CYS 862 19.922 43.756 9.943 1.00 27.50 ATOM 19.863 44.908 11.327 1.00 41.79 384 SG CYS 862 **ATOM** 21.876 42.424 9.146 1.00 25.51 -385 C CYS 862 **ATOM** 386 O CYS 862 21.241 41.492 8.700 1.00 30.38 ATOM **ATOM** 387 N ARG 863 23.136 42.307 9.541 1.00 27.68 MOTA 23.839 41.025 9.532 1.00 28.29 389 CA ARG 863 390 CB ARG 863 25.211 41.210 8.882 1.00 36.18 **ATOM** ATOM 391 CG ARG 863 25.775 39.945 8.275 1.00 48.71 27.282 40.034 7.943 1.00 58.46 MOTA 392 CD ARG 863 27.824 38.721 7.550 1.00 65.04 MOTA 393 NE ARG 863 395 CZ ARG 863 29.112 38.452 7.330 1.00 65.66 ATOM 29.482 37.219 6.985 1.00 67.60 396 NH1 ARG 863 **ATOM ATOM** 399 NH2 ARG 863 30.030 39.409 7.421 1.00 66.49 24.006 40.409 10.943 1.00 28.34 ATOM 402 C ARG 863 24.337 41.125 11.904 1.00 24.64 ATOM 403 O ARG 863 ATOM 404 N THR 864 23.735 39.100 11.078 1.00 23.23 406 CA THR 864 **MOTA** 23.900 38.426 12.364 1.00 18.91 23.062 37.099 12.489 1.00 19.40 **MOTA** 407 CB THR 864 ATOM 408 OG1 THR 864 21.672 37.435 12.547 1.00 24.20 23.371 36.351 13.793 1.00 8.83 MOTA 410 CG2 THR 864 25.385 38.148 12.462 1.00 20.93 MOTA 411 C THR 864 412 O THR 864 26.001 37.736 11.468 1.00 20.14 MOTA 413 N VAL 865 25.962 38.442 13.634 1.00 16.03 MOTA MOTA 415 CA VAL 865 27.381 38.254 13.897 1.00 16.69 28.175 39.620 13.906 1.00 17.70 416 CB VAL 865 MOTA 417 CG1 VAL 865 28.107 40.299 12.539 1.00 21.22 MOTA

FIG. 7(9)

418 CG2 VAL 865 27.625 40.554 14.979 1.00 20.92 ATOM 419 C VAL 865 27.533 37.660 15.276 1.00 15.90 ATOM 26.552 37.554 15.995 1.00 16.43 MOTA 420 O VAL 865 28.775 37.295 15.612 1.00 16.37 421 N ALA 866 ATOM **ATOM** 423 CA ALA 866 29.210 36.753 16.910 1.00 18.08 30.022 35.490 16.691 1.00 7.41 ATOM 424 CB ALA 866 425 C ALA 866 30.117 37.834 17.588 1.00 23.87 **MOTA** 31.121 38.261 16.998 1.00 24.17 ATOM 426 O ALA 866 29.790 38.235 18.827 1.00 26.69 427 N VAL 867 ATOM 30.534 39.268 19.554 1.00 20.37 **MOTA** 429 CA VAL 867 **MOTA** 430 CB VAL 867 29.592 40.365 20.088 1.00 17.71 30.361 41.586 20.519 1.00 9.32 431 CG1 VAL 867 MOTA 28.635 40.753 19.027 1.00 14.57 MOTA 432 CG2 VAL 867 31.320 38.748 20.728 1.00 21.67 ATOM 433 C VAL 867 30.784 38.085 21.606 1.00 23.57 434 O VAL 867 **MOTA** MOTA 435 N LYS 868 32.616 38.982 20.694 1.00 21.65 33.471 38.593 21.782 1.00 27.02 ATOM 437 CA LYS 868 34.860 38.169 21.289 1.00 29.71 438 CB LYS 868 **ATOM** 439 CG LYS 868 34.842 36.963 20.405 1.00 37.08 **ATOM** 36.151 36.810 19.666 1.00 44.81 440 CD LYS 868 ATOM ATOM 441 CE LYS 868 36.183 35.512 18.868 1.00 45.52 37.548 35.298 18.274 1.00 47.28 ATOM 442 NZ LYS 868 33.585 39.842 22.647 1.00 26.11 MOTA 446 C LYS 868 33.962 40.914 22.188 1.00 24.72 447 O LYS 868 ATOM 33.184 39.721 23.888 1.00 29.77 MOTA 448 N MET 869 33.299 40.821 24.803 1.00 32.95 450 CA MET 869 ATOM 31.958 41.491 24.996 1.00 30.57 ATOM 451 CB MET 869 30.900 40.542 25.463 1.00 32.29 452 CG MET 869 ATOM 29.348 41.157 24.961 1.00 42.68 **ATOM** 453 SD MET 869 MOTA 454 CE MET 869 29.251 42.663 25.919 1.00 35.32 33.778 40.205 26.095 1.00 40.29 MOTA 455 C MET 869 33.921 38.967 26.216 1.00 35.26 ATOM 456 O MET 869 34.079 41.066 27.051 1.00 46.88 ATOM 457 N LEU 870 34.521 40.576 28.337 1.00 51.36 ATOM 459 CA LEU 870 460 CB LEU 870 35.544 41.549 28.937 1.00 48.55 MOTA 36.862 41.677 28.180 1.00 44.32 MOTA 461 CG LEU 870 37.734 42.739 28.855 1.00 36.89 462 CD1 LEU 870 MOTA 37.535 40.306 28.149 1.00 41.04 MOTA 463 CD2 LEU 870 33.344 40.300 27.311 1.00 52.68 32.163 40.615 29.037 1.00 52.68 33.675 39.644 30.412 1.00 56.89 33.344 40.306 29.311 1.00 53.63 464 C LEU 870 MOTA MOTA 465 O LEU 870 MOTA 466 N LYS 871 32.695 39.346 31.426 1.00 58.53 468 CA LYS 871 MOTA 469 CB LYS 871 33.083 38.077 32.169 1.00 59.89 MOTA

FIG. 7(10)

470 CG LYS 871 MOTA 31.903 37.220 32.546 1.00 63.81 471 CD LYS 871 31.912 35.965 31.719 1.00 65.43 ATOM ATOM 472 CE LYS 871 33.268 35.318 31.853 1.00 70.59 473 NZ LYS 871 33.318 34.051 31.135 1.00 76.57 ATOM 477 C LYS 871 32.649 40.518 32.404 1.00 59.44 ATOM MOTA 478 O LYS 871 33.582 41.342 32.464 1.00 56.75 31.566 40.571 33.177 1.00 61.50 479 N GLU 872 ATOM MOTA 481 CA GLU 872 31.357 41.618 34.177 1.00 64.12 482 CB GLU 872 29.928 41.539 34.739 1.00 66.85 MOTA MOTA 483 CG GLU 872 28.846 41.903 33.729 1.00 71.27 484 CD GLU 872 29.060 41.218 32.387 1.00 74.41 ATOM 28.900 39.980 32.326 1.00 76.27 ATOM 485 OE1 GLU 872 486 OE2 GLU 872 29.443 41.903 31.411 1.00 74.20 ATOM **ATOM** 487 C GLU 872 32.387 41.424 35.288 1.00 60.87 ATOM 32.331 40.441 36.026 1.00 61.34 488 O GLU 872 489 N GLY 873 33.368 42.319 35.335 1.00 57.40 ATOM ATOM 491 CA GLY 873

 34.408
 42.223
 36.337
 1.00 53.93

 35.703
 41.641
 35.803
 1.00 52.30

 36.518
 41.103
 36.563
 1.00 51.95

 35.881
 41.721
 34.491
 1.00 51.13

 37.090
 41.217
 33.862
 1.00 51.21

 36.875
 41.049
 32.335
 1.00 48.57

 38.270
 42.172
 34.199
 1.00 50.40

 38.101
 43.388
 34.369
 1.00 48.57

 39.465
 41.609
 34.245
 1.00 48.33

 40.657
 42.334
 34.617
 1.00 51.59

 41.572
 41.428
 35.447
 1.00 54.42

 42.677
 42.184
 35.937
 1.00 60.69

 34.408 42.223 36.337 1.00 53.93 ATOM 492 C GLY 873 MOTA 493 O GLY 873 ATOM 494 N ALA 874 496 CA ALA 874 ATOM 497 CB ALA 874 MOTA ATOM 498 C ALA 874 **ATOM** 499 O ALA 874 MOTA 500 N THR 875 ATOM 502 CA THR 875 MOTA 503 CB THR 875 42.677 42.184 35.937 1.00 60.69 42.107 40.280 34.593 1.00 60.52 504 OG1 THR 875 MOTA MOTA 506 CG2 THR 875 507 C THR 875 41.455 42.830 33.448 1.00 51.15 MOTA

 41.395
 42.263
 32.372
 1.00 52.26

 42.343
 43.770
 33.733
 1.00 53.93

 43.215
 44.392
 32.737
 1.00 55.68

 44.170
 45.383
 33.419
 1.00 54.06

 45.609
 44.980
 33.361
 1.00 56.52

 46.595
 45.314
 32.487
 1.00 56.83

 46.191
 44.149
 34.297
 1.00 60.22

 47.472
 43.992
 34.009
 1.00 62.12

 47.739
 44.689
 32.916
 1.00 59.66

 44.003
 43.385
 31.898
 1.00 54.08

 44.510
 43.712
 30.810
 1.00 52.07

 44.872
 41.160
 31.704
 1.00 53.73

 41.395 42.263 32.372 1.00 52.26 ATOM 508 O THIR 875 ATOM 509 N HIS 876 511 CA HIS 876 MOTA ATOM 512 CB HIS 876 ATOM 513 CG HIS 876 **MOTA** 514 CD2 HIS 876 **MOTA** 515 ND1 HIS 876 MOTA 517 CE1 HIS 876 518 NE2 HIS 876 MOTA MOTA 520 C HIS 876 MOTA 521 O HIS 876 522 N SER 877 MOTA 524 CA SER 877 MOTA

FIG. 7(11)

525 CB SER 877 45.622 40.256 32.669 1.00 57.58 ATOM **ATOM** 526 OG SER 877 46.559 41.054 33.379 1.00 63.62 43.880 40.410 30.810 1.00 51.29 **ATOM** 528 C SER 877 529 O SER 877 44.227 39.962 29.715 1.00 50.11 MOTA 530 N GLU 878 42.629 40.320 31.246 1.00 47.72 ATOM 41.620 39.696 30.410 1.00 45.39 532 CA GLU 878 ATOM 40.335 39.483 31.201 1.00 48.19 533 CB GLU 878 MOTA 40.383 38.191 32.013 1.00 60.86 ATOM 534 CG GLU 878 39.304 38.086 33.092 1.00 68.27 535 CD GLU 878 ATOM 38.448 37.162 33.027 1.00 70.85 MOTA 536 OE1 GLU 878 39.336 38.911 34.029 1.00 67.92 MOTA 537 OE2 GLU 878 41.448 40.702 29.277 1.00 40.09 538 C GLU 878 **ATOM** 41.536 40.365 28.104 1.00 38.92 539 O GLU 878 ATOM **MOTA** 540 N HIS 879 41.393 41.966 29.659 1.00 34.60 41.252 43.072 28.732 1.00 36.68 542 CA HIS 879 MOTA 543 CB HIS 879 41.070 44.392 29.505 1.00 44.03 MOTA 40.637 45.547 28.652 1.00 43.54 544 CG HIS 879 ATOM 39.403 46.025 28.364 1.00 40.08 545 CD2 HIS 879 MOTA 546 ND1 HIS 879 41.529 46.307 27.917 1.00 39.08 ATOM ATOM 40.860 47.192 27.202 1.00 40.82 548 CE1 HIS 879 39.572 47.045 27.452 1.00 49.01 549 NE2 HIS 879 MOTA 42.455 43.172 27.797 1.00 34.17 42.293 43.494 26.626 1.00 33.65 551 C HIS 879 MOTA 552 O HIS 879 ATOM 43.664 42.993 28.319 1.00 33.25 ATOM 553 N ARG 880 44.838 43.033 27.470 1.00 29.84 MOTA 555 CA ARG 880 46.124 42.932 28.299 1.00 36.53 556 CB ARG 880 ATOM 557 CG ARG 880 46.615 41.470 28.452 1.00 50.57 MOTA 48.121 41.276 28.649 1.00 56.95 ATOM 558 CD ARG 880 48.555 41.748 29.960 1.00 63.99 559 NE ARG 880 ATOM 49.030 42.967 30.175 1.00 66.67 ATOM 561 CZ ARG 880 49.391 43.327 31.397 1.00 66.45 562 NH1 ARG 880 ATOM 49.170 43.813 29.157 1.00 66.52 MOTA 565 NH2 ARG 880 **MOTA** 568 C ARG 880 44.741 41.799 26.533 1.00 29.72 45.246 41.808 25.401 1.00 21.81 569 O ARG 880 MOTA 44.070 40.747 27.006 1.00 28.49 570 N ALA 881 MOTA 43.942 39.514 26.227 1.00 31.72 MOTA 572 CA ALA 881 573 CB ALA 881 43.587 38.342 27.142 1.00 31.57 MOTA 42.978 39.592 25.044 1.00 29.98 574 C ALA 881 MOTA 43.319 39.154 23.944 1.00 31.95 MOTA 575 O ALA 881 41.766 40.099 25.273 1.00 27.12 576 N LEU 882 MOTA MOTA 578 CA LEU 882 40.804 40.248 24.193 1.00 27.43 39.493 40.784 24.728 1.00 23.93 579 CB LEU 882 MOTA 38.402 40.925 23.662 1.00 25.91 580 CG LEU 882 MOTA

FIG. 7(12)

38.435 39.722 22.743 1.00 21.91 581 CD1 LEU 882 ATOM 37.013 41.102 24.325 1.00 23.61 582 CD2 LEU 882 ATOM 41.368 41.230 23.151 1.00 30.62 583 C LEU 882 ATOM 584 O LEU 882 41.312 40.982 21.945 1.00 27.61 MOTA 41.940 42.325 23.643 1.00 29.74 ATOM 585 N MET 883 42.548 43.364 22.808 1.00 30.75 587 CA MET 883 ATOM 588 CB MET 883 43.001 44.516 23.738 1.00 27.47 ATOM 43.432 45.828 23.084 1.00 33.64 589 CG MET 883 MOTA 590 SD MET 883 42.313 46.592 21.882 1.00 33.18 ATOM 41.031 47.285 22.943 1.00 33.54 **ATOM** 591 CE MET 883 43.711 42.756 21.965 1.00 29.92 592 C MET 883 ATOM 43.862 43.022 20.766 1.00 28.38 593 O MET 883 ATOM 44.501 41.893 22.588 1.00 29.75 ATOM 594 N SER 884 45.597 41.231 21.912 1.00 28.29 596 CA SER 884 ATOM 46.343 40.391 22.923 1.00 32.03 597 CB SER 884 ATOM 47.220 39.502 22.270 1.00 44.59 ATOM 598 OG SER 884 45.091 40.329 20.778 1.00 29.39 ATOM 600 C SER 884 601 O SER 884 45.595 40.359 19.654 1.00 28.92 ATOM 44.084 39.526 21.071 1.00 25.33 ATOM 602 N GLU 885 43.559 38.661 20.058 1.00 27.47 604 CA GLU 885 ATOM 605 CB GLU 885 42.563 37.692 20.661 1.00 31.61 ATOM 606 CG GLU 885 41.142 38.108 20.642 1.00 46.01 ATOM 40.215 36.903 20.799 1.00 55.19 ATOM 607 CD GLU 885 40.018 36.469 21.964 1.00 58.80 ATOM 608 OE1 GLU 885 39.715 36.379 19.762 1.00 54.01 609 OE2 GLU 885 ATOM 42.945 39.470 18.924 1.00 28.59 ATOM 610 C GLU 885 42.833 38.983 17.805 1.00 26.67 ATOM 611 O GLU 885 42.560 40.712 19.211 1.00 27.06 ATOM 612 N LEU 886 41.994 41.594 18.205 1.00 23.75 ATOM 614 CA LEU 886 41.483 42.887 18.847 1.00 22.79 ATOM 615 CB LEU 886 41.122 44.033 17.905 1.00 17.60 ATOM 616 CG LEU 886 617 CD1 LEU 886 39.981 43.608 16.999 1.00 11.98 ATOM 40.747 45.285 18.702 1.00 18.31 618 CD2 LEU 886 ATOM 43.049 41.936 17.147 1.00 24.77 619 C LEU 886 ATOM 42.767 41.880 15.939 1.00 22.15 MOTA 620 O LEU 886 44.265 42.246 17.602 1.00 25.08 621 N LYS 887 ATOM 623 CA LYS 887 45.384 42.613 16.722 1.00 24.94 ATOM 46.517 43.227 17.544 1.00 29.70 ATOM 624 CB LYS 887 46.105 44.304 18.560 1.00 30.67 625 CG LYS-887 MOTA 626 CD LYS 887 45.556 45.551 17.895 1.00 28.99 ATOM 45.170 46.645 18.923 1.00 26.07 627 CE LYS 887 MOTA 46.354 47.216 19.621 1.00 17.59 628 NZ LYS 887 ATOM 45.921 41.407 15.925 1.00 25.59 MOTA 632 C LYS 887

FIG. 7(13)

ATOM 633 O LYS 887 46.388 41.547 14.793 1.00 30.23 634 N ILE 888 45.917 40.235 16.542 1.00 20.48 **ATOM** ATOM 636 CA ILE 888 46.347 39.028 15.859 1.00 21.46 ATOM 637 CB ILE 888 46.306 37.795 16.816 1.00 22.73 638 CG2 ILE 888 46.604 36.556 16.047 1.00 24.05 ATOM 639 CG1 ILE 888 47.355 37.929 17.937 1.00 23.32 ATOM ATOM 640 CD1 ILE 888 47.092 37.058 19.190 1.00 18.29 ATOM 641 C ILE 888 45.392 38.822 14.663 1.00 19.51 642 O ILE 888 45.834 38.710 13.529 1.00 19.15 ATOM 643 N LEU 889 ATOM 44.088 38.828 14.922 1.00 15.54 43.078 38.677 13.872 1.00 20.73 ATOM 645 CA LEU 889 41.658 38.818 14.446 1.00 19.41 ATOM 646 CB LEU 889 647 CG LEU 889 41.204 37.652 15.372 1.00 22.61 ATOM **ATOM** 648 CD1 LEU 889 39.735 37.752 15.697 1.00 13.49 ATOM 649 CD2 LEU 889 41.500 36.263 14.764 1.00 18.87 ATOM 650 C LEU 889 43.308 39.678 12.762 1.00 24.12 **ATOM** 651 O LEU 889 43.342 39.344 11.584 1.00 28.65 **MOTA** 652 N ILE 890 43.461 40.931 13.138 1.00 29.62 654 CA ILE 890 43.753 41.953 12.158 1.00 26.41 ATOM 655 CB ILE 890 ATOM **- 43.966 43.310 12.865 1.00 24.45** ATOM 656 CG2 ILE 890 44.555 44.333 11.888 1.00 30.36 657 CG1 ILE 890 42.645 43.825 13.438 1.00 19.80 ATOM 658 CD1 ILE 890 42.812 45.061 14.241 1.00 14.93 ATOM ATOM 659 C ILE 890 45.053 41.519 11.415 1.00 28.37 ATOM 660 O ILE 890 45.126 41.553 10.191 1.00 24.83 661 N HIS 891 46.066 41.099 12.164 1.00 27.37 MOTA 663 CA HIS 891 47.309 40.659 11.567 1.00 27.76 MOTA ATOM 664 CB HIS 891 48.277 40.175 12.654 1.00 36.80 665 CG HIS 891 49.509 39.507 12.100 1.00 47.58 MOTA ATOM 666 CD2 HIS 891 50.811 39.869 12.147 1.00 46.38 667 ND1 HIS 891 49.450 38.394 11.276 1.00 52.71 ATOM ATOM 669 CE1 HIS 891 50.660 38.114 10.825 1.00 50.46 MOTA 670 NE2 HIS 891 51.505 38.993 11.340 1.00 54.62 672 C HIS 891 47.098 39.536 10.537 1.00 27.01 MOTA 47.522 39.647 9.402 1.00 32.82 673 O HIS 891 MOTA 46.580 38.403 10.995 1.00 24.99 ATOM 674 N ILE 892 MOTA 676 CA ILE 892 46.300 37.216 10.181 1.00 23.19 677 CB ILE 892 45.233 36.282 10.907 1.00 24.73 MOTA 44.643 35.295 9.941 1.00 20.03 45.828 35.522 12.104 1.00 26.32 47.015 36.222 12.787 1.00 36.72 ATOM 678 CG2 ILE 892 679 CG1 ILE 892 ATOM ATOM 680 CD1 ILE 892 45.700 37.625 8.848 1.00 22.57 681 C ILE 892 MOTA 46.115 37.155 7.775 1.00 25.20 ATOM 682 O ILE 892

FIG. 7(14)

ATOM	683 N GLY 893	44.699 38.492	8.916 1.00 23.88
ATOM	685 CA GLY 893	44.034 38.910	7.702 1.00 25.37
ATOM	686 C GLY 893	42.794 38.080	7.403 1.00 25.54
ATOM	687 O GLY 893	42.303 37.326	8.224 1.00 32.60
ATOM	688 N HIS 894	42.327 38.149	6.176 1.00 26.97
ATOM	690 CA HIS 894	41.120 37.457	5.797 1.00 26.35
ATOM	691 CB HIS 894	40.233 38.464	5.042 1.00 31.72
ATOM	692 CG HIS 894	39.114 37.833	4.274 1.00 35.68
ATOM	693 CD2 HIS 894	37.818 37.609	4.608 1.00 34.18
ATOM	694 ND1 HIS 894	39.271 37.346	2.989 1.00 38.36
ATOM	696 CE1 HIS 894	38.121 36.854	2.568 1.00 36.24
ATOM	697 NE2 HIS 894	37.224 37.004	3.527 1.00 35.86
ATOM	699 C HIS 894	41.253 36.182	4.958 1.00 24.38
ATOM	700 O HIS 894	42.045 36.108	4.007 1.00 24.24
ATOM	701 N HIS 895	40.426 35.202	5.280 1.00 17.00
ATOM	703 CA HIS 895	40.379 33.994	4.494 1.00 18.62
ATOM	704 CB HIS 895	41.363 32.929	4.931 1.00 15.85
ATOM	705 CG HIS 895	41.446 31.814	3.943 1.00 21.47
ATOM	706 CD2 HIS 895	42.076 31.737	2.745 1.00 17.93
ATOM	707 ND1 HIS 895	40.675 30.676	4.042 1.00 21.96
ATOM	709 CE1 HIS 895	40.819 29.956	2.938 1.00 21.22
ATOM	710 NE2 HIS 895	41.663 30.578	2.137 1.00 10.16
ATOM	712 C HIS 895	38.979 33.467	4.626 1.00 15.66
ATOM	713 O HIS 895	38.396 33.656	5.663 1.00 18.76
ATOM	714 N LEU 896	38.419 32.865	3.567 1.00 21.74
ATOM	716 CA LEU 896	37.042 32.306	3.584 1.00 18.37
MOTA	717 CB LEU 896	36.652 31.762	2.210 1.00 17.64
MOTA	718 CG LEU 896	35.297 31.068	2.218 1.00 25.15
ATOM	719 CD1 LEU 896	34.218 32.077	2.454 1.00 24.41
MOTA	720 CD2 LEU 896	35.042 30.342	0.934 1.00 25.59
MOTA	721 C LEU 896	36.867 31.172	4.569 1.00 17.58
MOTA	722 O LEU 896	35.783 30.937	5.068 1.00 23.11
MOTA	723 N ASN 897	37.952 30.475	4.849 1.00 15.99
MOTA	725 CA ASN 897		5.725 1.00 18.36
ATOM	726 CB ASN 897		5.078 1.00 20.86
MOTA	727 CG ASN 897		3.747 1.00 16.88
MOTA	728 OD1 ASN 897	38.567 27.692	2.694 1.00 14.51
MOTA	729 ND2 ASN 897	36.639 27.346	3.799 1.00 12.11
ATOM	732 C ASN 897	38.293 29.541	7.188 1.00 25.65
ATOM	733 O ASN 897	38.648 28.556	7.858 1.00 22.22
MOTA	734 N VAL 898		7.660 1.00 23.53
ATOM	736 CA VAL 898		9.081 1.00 15.38
MOTA	737 CB VAL 898	40.036 31.719	9.457 1.00 11.47

FIG. 7(15)

MOTA 738 CG1 VAL 898 41.146 30.813 9.017 1.00 14.76 739 CG2 VAL 898 40.236 33.119 8.883 1.00 8.71 ATOM 37.475 31.959 9.477 1.00 15.57 **ATOM** 740 C VAL 898 741 O VAL 898 36.698 32.382 8.620 1.00 17.87 ATOM 37.226 32.049 10.773 1.00 18.55 742 N VAL 899 ATOM 744 CA VAL 899 36.155 32.882 11.264 1.00 20.68 ATOM 35.757 32.487 12.720 1.00 19.98 ATOM 745 CB VAL 899 746 CG1 VAL 899 34.618 33.384 13.202 1.00 18.29 ATOM 747 CG2 VAL 899 35.346 31.016 12.788 1.00 12.67 ATOM 36.807 34.272 11.244 1.00 21.95 748 C VAL 899 MOTA 749 O VAL 899 37.725 34.517 12.003 1.00 21.42 **ATOM** 36.352 35.164 10.363 1.00 23.43 750 N ASN 900 **ATOM** 36.930 36.526 10.226 1.00 23.52 **MOTA** 752 CA ASN 900 36.737 37.061 8.803 1.00 19.45 753 CB ASN 900 ATOM 754 CG ASN 900 37.350 36.177 7.782 1.00 19.58 ATOM 38.578 36.087 7.667 1.00 17.65 ATOM 755 OD1 ASN 900 36.511 35.528 7.004 1.00 20.34 MOTA 756 ND2 ASN 900 36.484 37.641 11.152 1.00 17.00 759 C ASN 900 ATOM 35.343 37.704 11.598 1.00 16.94 760 O ASN 900 ATOM 37.413 38.544 11.384 1.00 17.25 761 N LEU 901 MOTA 763 CA LEU 901 37.167 39.733 12.160 1.00 17.98 ATOM 764 CB LEU 901 38.494 40.447 12.426 1.00 16.80 ATOM 38.444 41.819 13.101 1.00 14.17 765 CG LEU 901 MOTA MOTA 766 CD1 LEU 901 38.018 41.673 14.560 1.00 11.71 767 CD2 LEU 901 39.782 42.435 13.008 1.00 2.76 **ATOM** 36.354 40.578 11.174 1.00 20.28 768 C LEU 901 ATOM MOTA 769 O LEU 901 36.669 40.612 9.965 1.00 18.06 770 N LEU 902 35.280 41.180 11.686 1.00 19.74 MOTA 772 CA LEU 902 34.398 42.031 10.917 1.00 15.84 **MOTA** 773 CB LEU 902 32.950 41.593 11.087 1.00 11.70 ATOM 32.615 40.230 10.473 1.00 13.49 **ATOM** 774 CG LEU 902 775 CD1 LEU 902 31.142 39.827 10.774 1.00 13.78 MOTA 32.856 40.270 8.981 1.00 12.15 ATOM 776 CD2 LEU 902 777 C LEU 902 34.566 43.486 11.345 1.00 19.59 MOTA 34.466 44.380 10.510 1.00 23.95 ATOM 778 O LEU 902 779 N GLY 903 34.854 43.724 12.625 1.00 20.15 MOTA 35.037 45.090 13.114 1.00 21.60 **ATOM** 781 CA GLY 903 35.147 45.075 14.620 1.00 24.02 ATOM 782 C GLY 903 35.070 43.991 15.194 1.00 26.53 ATOM 783 O GLY 903 784 N ALA 904 35.305 46.236 15.269 1.00 25.19 MOTA 35.411 46.293 16.740 1.00 18.80 MOTA 786 CA ALA 904 787 CB ALA 904 36.830 46.074 17.177 1.00 12.62 MOTA 34.886 47.559 17.386 1.00 20.83 788 C ALA 904 MOTA

FIG. 7(16)

789 O ALA 904 34.789 48.616 16.765 1.00 26.12 ATOM MOTA 790 N CYS 905 34.617 47.443 18.674 1.00 21.21 34.128 48.530 19.493 1.00 19.91 **ATOM** 792 CA CYS 905 **ATOM** 793 CB CYS 905 32.804 48.160 20.115 1.00 16.08 794 SG CYS 905 31.561 47.894 18.851 1.00 15.32 ATOM 795 C CYS 905 35.176 48.687 20.556 1.00 23.00 ATOM 796 O CYS 905 35.245 47.890 21.486 1.00 24.21 MOTA 36.042 49.674 20.361 1.00 26.02 ATOM 797 N THR 906 799 CA THR 906 37.140 49.945 21.283 1.00 29.46 MOTA 800 CB THR 906 38.514 49.768 20.574 1.00 26.67 **ATOM** 38.635 50.739 19.526 1.00 29.06 801 OG1 THR 906 ATOM 803 CG2 THR 906 38.648 48.363 20.001 1.00 23.13 **ATOM** 37.130 51.346 21.928 1.00 30.07 804 C THR 906 ATOM 37.642 51.522 23.036 1.00 29.29 805 O THR 906 ATOM 36.582 52.332 21.228 1.00 32.81 806 N LYS 907 ATOM ATOM 808 CA LYS 907 36.554 53.686 21.745 1.00 39.38 35.982 54.637 20.701 1.00 41.03 **MOTA** 809 CB LYS 907 810 CG LYS 907 34.536 54.432 20.386 1.00 48.86 ATOM 811 CD LYS 907 34.071 55.528 19.427 1.00 57.25 ATOM 33.996 56.878 20.143 1.00 63.62 ATOM 812 CE LYS 907 813 NZ LYS 907 33.688 58.001 19.213 1.00 68.81 ATOM 35.796 53.779 23.070 1.00 44.43 ATOM 817 C LYS 907 35.094 52.867 23.442 1.00 44.52 818 O LYS 907 ATOM MOTA 819 N PRO 908 36.034 54.838 23.857 1.00 49.18 37.147 55.794 23.712 1.00 50.93 820 CD PRO 908 ATOM 35.358 55.022 25.149 1.00 46.86 821 CA PRO 908 MOTA **ATOM** 822 CB PRO 908 35.963 56.324 25.647 1.00 49.68 37.387 56.216 25.143 1.00 51.43 MOTA 823 CG PRO 908 **ATOM** 824 C PRO 908 33.852 55.145 25.036 1.00 44.06 33.345 55.600 24.008 1.00 44.40 MOTA 825 O PRO 908 33.154 54.772 26.110 1.00 41.44 **MOTA** 826 N GLY 909 828 CA GLY 909 31.698 54.842 26.135 1.00 37.38 MOTA 829 C GLY 909 30.999 53.502 26.035 1.00 38.26 MOTA 830 O GLY 909 29.778 53.439 25.751 1.00 40.07 MOTA MOTA 831 N GLY 910 31.753 52.424 26.264 1.00 36.39 31.178 51.087 26.190 1.00 34.35 MOTA 833 CA GLY 910 32.180 49.961 26.360 1.00 31.85 834 C GLY 910 MOTA 33.394 50.235 26.528 1.00 27.95 835 O GLY 910 MOTA 31.710 48.686 26.319 1.00 27.95 836 N PRO 911 MOTA 30.280 48.339 26.197 1.00 28.51 MOTA 837 CD PRO 911 32.511 47.463 26.467 1.00 25.21 838 CA PRO 911 MOTA 31.438 46.393 26.724 1.00 27.44 MOTA 839 CB PRO 911 30.315 46.840 25.891 1.00 22.45 840 CG PRO 911 MOTA

FIG. 7(17)

ATOM 841 C PRO 911 33.340 47.118 25.234 1.00 22.33 34.548 46.581 25.430 1.00 23.57 35.412 46.177 24.308 1.00 23.22 36.778 45.685 24.812 1.00 23.23 38.095 45.750 **ATOM** 842 O PRO 911 **ATOM** 843 N LEU 912 ATOM 845 CA LEU 912 846 CB LEU 912 ATOM ATOM 847 CG LEU 912 **ATOM** 848 CD1 LEU 912 38.988 44.618 24.490 1.00 20.11 38.988 44.618 24.490 1.00 20.11 37.906 45.745 22.477 1.00 12.72 849 CD2 LEU 912 **ATOM** MOTA 850 C LEU 912 34.692 45.010 23.627 1.00 22.56 34.342 44.029 24.283 1.00 17.69
34.417 45.142 22.334 1.00 24.19
33.724 44.085 21.617 1.00 21.51
32.264 44.456 21.429 1.00 22.09
31.489 44.461 22.728 1.00 22.26
29.829 45.009 22.484 1.00 24.17
30.127 46.676 22.205 1.00 20.40 ATOM 851 O LEU 912 **ATOM** 852 N MET 913 **MOTA** 854 CA MET 913 ATOM 855 CB MET 913 ATOM 856 CG MET 913 **ATOM** 857 SD MET 913 858 CE MET 913 **MOTA** 30.127 46.676 22.205 1.00 20.40
34.386 43.768 20.295 1.00 20.42
34.701 44.657 19.519 1.00 21.08
34.703 42.491 20.102 1.00 23.72
35.354 42.001 18.891 1.00 20.24
36.614 41.170 19.232 1.00 16.92
37.254 40.637 17.958 1.00 19.36
37.629 42.055 19.972 1.00 13.30
34.296 41.210 18.132 1.00 19.70
33.836 40.191 18.587 1.00 26.45
33.844 41.775 17.026 1.00 19.86
32.806 41.212 16.179 1.00 20.42
32.034 42.384 15.455 1.00 18.44
30.721 41.909 14.869 1.00 12.35
31.756 43.531 16.426 1.00 17.60
31.358 44.822 15.735 1.00 15.14
33.457 40.287 15.115 1.00 23.98
34.361 40.722 14.373 1.00 23.30
33.054 39.011 15.075 1.00 20.08
33.594 38.089 14.077 1.00 17.64
34.543 37.003 14.680 1.00 9.09
35.703 37.685 15.350 1.00 5.05
33.817 36.126 15.678 1.00 10.26
32.422 37.486 13.342 1.00 17.74
31.275 37.790 13.664 1.00 20.02
32.684 36.702 12.303 1.00 14.74
31.589 36.073 11.577 1.00 13.03
32.120 35.409 10.332 1.00 14.06 34.386 43.768 20.295 1.00 20.42 ATOM 859 C MET 913 ATOM 860 O MET 913 ATOM 861 N VAL 914 863 CA VAL 914 ATOM ATOM 864 CB VAL 914 865 CG1 VAL 914 ATOM ATOM 866 CG2 VAL 914 ATOM 867 C VAL 914 868 O VAL 914 **ATOM MOTA** 869 N ILE 915 MOTA 871 CA ILE 915 MOTA 872 CB ILE 915 MOTA 873 CG2 ILE 915 ATOM 874 CG1 ILE 915 ATOM 875 CD1 ILE 915 876 C ILE 915 MOTA MOTA 877 O ILE 915 MOTA 878 N VAL 916 880 CA VAL 916 MOTA MOTA 881 CB VAL 916 MOTA 882 CG1 VAL 916 MOTA 883 CG2 VAL 916 MOTA 884 C VAL 916 MOTA 885 O VAL 916 MOTA 886 N GLU 917 ATOM 888 CA GLU 917 MOTA 889 CB GLU 917

FIG. 7(18)

890 CG GLU 917 32.946 36.348 9.464 1.00 24.11 ATOM **MOTA** 891 CD GLU 917 33.543 35.651 8.258 1.00 26.52 ATOM 892 OE1 GLU 917 33.060 35.904 7.139 1.00 27.67 **MOTA** 893 OE2 GLU 917 34.480 34.841 8.425 1.00 28.39 ATOM 894 C GLU 917 30.853 35.051 12.434 1.00 14.78 895 O GLU 917 31.445 34.344 13.234 1.00 14.35 ATOM 896 N PHE 918 29.557 34.958 12.229 1.00 19.12 ATOM 28.688 34.042 12.966 1.00 18.07 ATOM 898 CA PHE 918 28.688 34.042 12.966 1.00 18.07 27.334 34.721 13.168 1.00 18.48 MOTA 899 CB PHE 918 900 CG PHE 918 26.275 33.840 13.748 1.00 17.83 MOTA 901 CD1 PHE 918 26.328 33.456 15.081 1.00 18.65 **ATOM** 25.213 33.400 12.953 1.00 21.10 ATOM 902 CD2 PHE 918 ATOM 903 CE1 PHE 918 25.336 32.639 15.613 1.00 18.12 904 CE2 PHE 918 24.210 32.580 13.473 1.00 14.29 ATOM ATOM 905 CZ PHE 918 24.274 32.201 14.799 1.00 17.78 ATOM 906 C PHE 918 28.487 32.805 12.113 1.00 18.83 **ATOM** 907 O PHE 918 28.081 32.917 10.964 1.00 11.61 28.761 31.635 12.676 1.00 19.49 28.590 30.372 11.947 1.00 19.00 908 N CYS 919 ATOM ATOM 910 CA CYS 919 29.855 29.566 12.069 1.00 16.78 ATOM 911 CB CYS 919 ATOM 912 SG CYS 919 31.225 30.428 11.325 1.00 16.84 913 C CYS 919 27.383 29.659 12.556 1.00 21.18 ATOM ATOM 914 O CYS 919 27.474 29.135 13.676 1.00 20.69 ATOM 915 N LYS 920 26.269 29.653 11.818 1.00 18.06 ATOM 917 CA LYS 920 24.998 29.130 12.318 1.00 28.13 23.799 29.581 11.459 1.00 25.17 918 CB LYS 920 ATOM ATOM 919 CG LYS 920 23.595 28.799 10.207 1.00 33.78 920 CD LYS 920 22.658 29.509 9.250 1.00 40.32 ATOM ATOM 921 CE LYS 920 21.261 29.706 9.829 1.00 51.94 20.343 30.396 8.845 1.00 56.09 ATOM 922 NZ LYS 920 24.813 27.679 12.700 1.00 28.53 ATOM 926 C LYS 920 927 O LYS 920 24.020 27.405 13.592 1.00 31.57 MOTA 928 N PHE 921 25.533 26.757 12.078 1.00 24.89 MOTA 930 CA PHE 921 25.328 25.362 12.409 1.00 21.12 MOTA ATOM 931 CB PHE 921 25.497 24.518 11.171 1.00 20.75 ATOM 932 CG PHE 921 24.588 24.917 10.084 1.00 22.95 MOTA 933 CD1 PHE 921 23.224 24.734 10.219 1.00 27.55 934 CD2 PHE 921 25.077 25.564 8.975 1.00 29.40 MOTA 935 CE1 PHE 921 22:362 25.205 9.269 1.00 35.42 ATOM 24.237 26.041 8.013 1.00 32.24 MOTA 936 CE2 PHE 921 937 CZ PHE 921 22.869 25.870 8.154 1.00 38.81 ATOM ATOM 938 C PHE 921 26.158 24.823 13.535 1.00 21.23 26.002 23.664 13.900 1.00 22.74 ATOM 939 O PHE 921

FIG. 7(19)

ATOM 940 N GLY 922 27.047 25.659 14.065 1.00 18.39 ATOM 27.906 25.257 15.172 1.00 17.62 942 CA GLY 922 29.115 24.455 14.759 1.00 18.42 ATOM 943 C GLY 922 ATOM 944 O GLY 922 29.331 24.230 13.581 1.00 20.81 ATOM 945 N ASN 923 29.903 24.011 15.729 1.00 22.93 MOTA 947 CA ASN 923 31.092 23.223 15.430 1.00 24.85 948 CB ASN 923 31.867 22.837 16.705 1.00 29.68 ATOM 949 CG ASN 923 31.212 21.710 17.493 1.00 39.14 ATOM 950 OD1 ASN 923 31.252 20.550 17.087 1.00 41.11 ATOM ATOM 951 ND2 ASN 923 30.662 22.038 18.660 1.00 35.87 954 C ASN 923 30.818 22.019 14.523 1.00 21.09 ATOM ATOM 955 O ASN 923 29.685 21.566 14.370 1.00 20.59 MOTA 956 N LEU 924 31.867 21.523 13.896 1.00 21.13 ATOM 958 CA LEU 924 31.740 20.431 12.957 1.00 22.85 MOTA 959 CB LEU 924 33.019 20.377 12.126 1.00 23.67 960 CG LEU 924 33.019 19.462 10.920 1.00 17.22 ATOM 961 CD1 LEU 924 31.776 19.699 10.125 1.00 18.21 MOTA 962 CD2 LEU 924 34.268 19.729 10.095 1.00 23.82 MOTA 963 C LEU 924 31.414 19.062 13.558 1.00 22.65 ATOM 964 O LEU 924 30.601 18.326 13.013 1.00 26.13 ATOM MOTA 965 N SER 925 31.035 18.742 14.687 1.00 20.06 967 CA SER 925 31.853 17.463 15.383 1.00 25.99 ATOM ATOM 968 CB SER 925 32.741 17.400 16.623 1.00 27.28 969 OG SER 925 32.426 16.272 17.416 1.00 32.86 **ATOM** 971 C SER 925 30.432 17.217 15.812 1.00 26.73 ATOM ATOM 972 O SER 925 29.863 16.148 15.552 1.00 30.93 973 N THR 926 29.892 18.190 16.534 1.00 24.48 ATOM 975 CA THR 926 ATOM 28.535 18.129 16.996 1.00 19.27 976 CB THR 926 28.258 19.336 17.901 1.00 16.05 ATOM MOTA 977 OG1 THR 926 29.230 19.374 18.951 1.00 18.42 ATOM 979 CG2 THR 926 26.927 19.216 18.550 1.00 13.93 980 C THR 926 27.610 18.048 15.758 1.00 20.47 MOTA 981 O THR 926 26.654 17.258 15.711 1.00 25.12 ATOM MOTA 982 N TYR 927 27.961 18.760 14.701 1.00 18.97 984 CA TYR 927 27.128 18.715 13.515 1.00 20.97 MOTA MOTA 985 CB TYR 927 27.597 19.720 12.464 1.00 18.52 MOTA 986 CG TYR 927 26.708 19.683 11.230 1.00 18.69 987 CD1 TYR 927 25.391 20.196 11.266 1.00 14.64 MOTA MOTA 988 CE1 TYR 927 24.567 20.173 10.125 1.00 13.73 989 CD2 TYR 927 27.173 19.138 10.031 1.00 22.28 MOTA MOTA 990 CE2 TYR 927 26.347 19.104 8.879 1.00 24.92 991 CZ TYR 927 25.058 19.626 8.944 1.00 16.40 MOTA MOTA 992 OH TYR 927 24.285 19.600 7.819 1.00 23.87

FIG. 7(20)

ATOM 994 C TYR 927 27.118 17.343 12.855 1.00 23.85 ATOM 995 O TYR 927 26.078 16.860 12.428 1.00 24.11 996 N LEU 928 ATOM 28.313 16.793 12.665 1.00 28.91 ATOM 998 CA LEU 928 28.513 15.495 12.020 1.00 31.09 999 CB LEU 928 ATOM 30.017 15.192 11.863 1.00 27.50 ATOM 1000 CG LEU 928 30.813 16.159 10.953 1.00 24.21 ATOM 1001 CD1 LEU 928 32.302 15.880 11.065 1.00 24.38 30.343 16.097 9.514 1.00 12.63 27.801 14.369 12.747 1.00 31.00 27.164 13.540 12.117 1.00 31.53 27.883 14.351 14.067 1.00 34.05 27.193 13.316 14.833 1.00 40.50 27.406 13.552 16.325 1.00 41.71 28.358 12.605 16.969 1.00 40.42 29.253 13.359 17.908 1.00 49.36 28.521 13.947 19.020 1.00 62.28 28.946 14.985 19.749 1.00 65.86 ATOM 1002 CD2 LEU 928 30.343 16.097 9.514 1.00 12.63 ATOM 1003 C LEU 928 ATOM 1004 O LEU 928 ATOM 1005 N ARG 929 ATOM 1007 CA ARG 929 ATOM 1008 CB ARG 929 ATOM 1009 CG ARG 929 ATOM 1010 CD ARG 929 ATOM 1011 NE ARG 929 ATOM 1013 CZ ARG 929 28.178 15.432 20.753 1.00 58.39 30.122 15.573 19.492 1.00 58.39 25.678 13.304 14.529 1.00 42.76 ATOM 1014 NH1 ARG 929 ATOM 1017 NH2 ARG 929 ATOM 1020 C ARG 929

 - 25.678
 13.304
 14.529
 1.00 42.76

 25.075
 12.234
 14.370
 1.00 44.84

 25.089
 14.498
 14.412
 1.00 41.42

 23.663
 14.677
 14.150
 1.00 37.04

 23.324
 16.151
 14.250
 1.00 38.80

 23.662
 16.816
 13.041
 1.00 37.58

 23.226
 14.226
 12.774
 1.00 38.41

 22.034
 14.254
 12.451
 1.00 43.98

 24.179
 13.865
 11.936
 1.00 37.60

 23.845
 13.472
 10.590
 1.00 38.82

 24.575
 14.387
 9.606
 1.00 43.10

 24.388
 15.864
 9.884
 1.00 45.62

 ATOM 1021 O ARG 929 ATOM 1022 N SER 930 ATOM 1024 CA SER 930 ATOM 1025 CB SER 930 ATOM 1026 OG SER 930 ATOM 1028 C SER 930 ATOM 1029 O SER 930 ATOM 1030 N LYS 931 ATOM 1032 CA LYS 931 ATOM 1033 CB LYS 931 ATOM 1034 CG LYS 931 24.388 15.864 9.884 1.00 45.62 ATOM 1035 CD LYS 931 22.999 16.302 9.487 1.00 49.49 ATOM 1036 CE LYS 931 22.901 16.444 7.985 1.00 46.94 ATOM 1037 NZ LYS 931 21.501 16.690 7.568 1.00 49.54 ATOM 1041 C LYS 931 24.136 12.011 10.264 1.00 39.02

 24.136
 12.011
 10.20

 23.991
 11.615
 9.111
 1.00 42.79

 24.522
 11.199
 11.247
 1.00 37.44

 24.793
 9.776
 10.971
 1.00 38.33

 25.149
 9.020
 12.244
 1.00 33.55

 26.456
 9.461
 12.798
 1.00 33.92

 26.812
 8.729
 14.043
 1.00 35.88

 28.223
 8.929
 14.368
 1.00 43.26

 28.720
 8.909
 15.604
 1.00 45.56

 ATOM 1042 O LYS 931 ATOM 1043 N ARG 932 ATOM 1045 CA ARG 932 ATOM 1046 CB ARG 932 ATOM 1047 CG ARG 932 ATOM 1048 CD ARG 932 ATOM 1049 NE ARG 932 ATOM 1051 CZ ARG 932

FIG. 7(21)

ATOM 1052 NH1 ARG 932 30.018 9.098 15.809 1.00 47.32 ATOM 1055 NH2 ARG 932 27.916 8.725 16.645 1.00 53.04 ATOM 1058 C ARG 932 23.621 9.087 10.273 1.00 41.54 23.621 9.087 10.273 1.00 41.54
23.821 8.135 9.532 1.00 41.31
22.412 9.582 10.536 1.00 44.37
21.181 9.069 9.956 1.00 47.14
19.974 9.453 10.824 1.00 54.55
19.783 8.545 12.050 1.00 57.14
20.622 7.693 12.369 1.00 54.11
18.668 8.752 12.757 1.00 57.76
20.974 9.680 8.589 1.00 49.60
20.260 9.125 7.753 1.00 55.62
21.494 10.888 8.403 1.00 52.11
21.365 11.580 7.122 1.00 52.39
20.859 13.007 7.323 1.00 56.14
19.434 13.095 7.822 1.00 59.40
19.332 13.686 9.211 1.00 63.97
18.427 13.250 9.953 1.00 69.17
20.138 14.580 9.563 1.00 64.27
22.677 11.593 6.332 1.00 50.45
23.188 12.663 5.961 1.00 50.70
23.205 10.396 6.070 1.00 46.25
24.440 10.225 5.325 1.00 41.20
25.638 10.121 6.268 1.00 40.97
26.923 9.800 5.555 1.00 39.81
27.327 8.478 5.378 1.00 34.65
27.676 10.815 4.970 1.00 33.02
28.455 8.180 4.617 1.00 32.30
28.793 10.515 4.218 1.00 29.96
29.181 9.201 4.037 1.00 29.08
24.474 9.006 4.412 1.00 40.49
24.394 7.871 4.865 1.00 40.47
24.694 9.237 3.133 1.00 38.66
24.809 8.138 2.208 1.00 43.29 23.821 8.135 9.532 1.00 41.31 ATOM 1059 O ARG 932 ATOM 1060 N ASN 933 ATOM 1062 CA ASN 933 ATOM 1063 CB ASN 933 ATOM 1064 CG ASN 933 ATOM 1065 OD1 ASN 933 ATOM 1066 ND2 ASN 933 ATOM 1069 C ASN 933 ATOM 1070 O ASN 933 ATOM 1071 N GLU 934 ATOM 1073 CA GLU 934 ATOM 1074 CB GLU 934 ATOM 1075 CG GLU 934 ATOM 1076 CD GLU 934 ATOM 1077 OE1 GLU 934 ATOM 1078 OE2 GLU 934 ATOM 1079 C GLU 934 ATOM 1080 O GLU 934 ATOM 1081 N PHE 935 ATOM 1083 CA PHE 935 ATOM 1084 CB PHE 935 ATOM 1085 CG PHE 935 ATOM 1086 CD1 PHE 935 ATOM 1087 CD2 PHE 935 ATOM 1088 CE1 PHE 935 ATOM 1089 CE2 PHE 935 ATOM 1090 CZ PHE 935 ATOM 1091 C PHE 935 ATOM 1092 O PHE 935 ATOM 1093 N VAL 936 24.694 9.237 3.133 1.00 38.66

 24.694
 9.237
 3.133
 1.00 38.66

 24.809
 8.138
 2.208
 1.00 43.29

 23.663
 8.113
 1.221
 1.00 40.39

 23.739
 9.312
 0.280
 1.00 34.50

 23.720
 6.841
 0.444
 1.00 42.47

 26.087
 8.436
 1.438
 1.00 49.63

 26.322
 9.585
 1.081
 1.00 55.64

 26.960
 7.433
 1.222
 1.00 50.29

 26.966
 6.087
 1.822
 1.00 49.69

 28.207
 7.669
 0.483
 1.00 50.65

 28.676
 6.260
 0.177
 1.00 46.68

 ATOM 1095 CA VAL 936 ATOM 1096 CB VAL 936 ATOM 1097 CG1 VAL 936 ATOM 1098 CG2 VAL 936 ATOM 1099 C VAL 936 ATOM 1100 O VAL 936 ATOM 1101 N PRO 937 ATOM 1102 CD PRO 937 ATOM 1103 CA PRO 937 ATOM 1104 CB PRO 937

FIG. 7(22)

ATOM 1105 CG PRO 937 28.378 5.582 1.493 1.00 47.42 ATOM 1106 C PRO 937 28.019 8.501 -0.774 1.00 53.83 ATOM 1107 O PRO 937 28.644 9.558 -0.937 1.00 53.64 ATOM 1108 N TYR 938 27.153 8.046 -1.660 1.00 54.91 ATOM 1110 CA TYR 938 26.918 8.803 -2.859 1.00 62.52 ATOM 1111 CB TYR 938 27.580 8.161 -4.080 1.00 67.73 ATOM 1120 C TYR 938 25.443 8.800 -3.059 1.00 67.31 ATOM 1121 O TYR 938 24.722 8.082 -2.361 1.00 66.13 ATOM 1122 N LYS 939 25.027 9.601 -4.038 1.00 75.30 ATOM 1124 CA LYS 939 23.639 9.770 -4.445 1.00 81.21 23.209 11.254 -4.284 1.00 80.04 23.543 9.331 -5.921 1.00 87.24 23.639 9.770 -4.445 1.00 81.21 ATOM 1125 CB LYS 939 ATOM 1126 C LYS 939 ATOM 1127 O LYS 939 24.582 9.384 -6.646 1.00 90.23 ATOM 1129 CB ASP 998 17.986 15.692 3.023 1.00 53.00 ATOM 1130 C ASP 998 20.489 15.723 3.377 1.00 55.33 ATOM 1131 O ASP 998 21.051 16.058 4.426 1.00 56.29 ATOM 1134 N ASP 998 19.408 16.931 1.400 1.00 54.52 19.279 16.514 2.829 1.00 55.12 ATOM 1136 CA ASP 998 ATOM 1137 N PHE 999 20.900 14.687 2.653 1.00 52.90 ATOM 1139 CA PHE 999 21.984 13.834 3.111 1.00 46.86 ATOM 1140 CB PHE 999 21.841 12.420 2.528 1.00 51.05 ATOM 1141 CG PHE 999 20.897 11.537 3.296 1.00 55.62 ATOM 1142 CD1 PHE 999 21.249 10.236 3.606 1.00 56.12 ATOM 1143 CD2 PHE 999 19.671 12.022 3.751 1.00 60.98 ATOM 1144 CE1 PHE 999 20.397 9.422 4.368 1.00 61.93 ATOM 1145 CE2 PHE 999 18.816 11.222 4.509 1.00 61.09 ATOM 1146 CZ PHE 999 19.183 9.917 4.820 1.00 60.64 ATOM 1147 C PHE 999 23.373 14.302 2.837 1.00 41.06 23.632 14.937 1.820 1.00 36.04 ATOM 1148 O PHE 999 ATOM 1149 N LEU 1000 24.238 14.057 3.812 1.00 37.57 ATOM 1151 CA LEU 1000 25.651 14.326 3.652 1.00 36.08 26.401 14.306 4.985 1.00 35.67 ATOM 1152 CB LEU 1000 ATOM 1153 CG LEU 1000 25.923 15.286 6.057 1.00 36.23 ATOM 1154 CD1 LEU 1000 26.941 15.370 7.201 1.00 29.94 ATOM 1155 CD2 LEU 1000 25.707 16.654 5.435 1.00 38.66 ATOM 1156 C LEU 1000 26.089 13.139 2.756 1.00 35.16 ATOM 1157 O LEU 1000 25.339 12.167 2.569 1.00 32.68 27.292 13.228 2.201 1.00 25.42 27.803 12.236 1.285 1.00 25.42 27.396 12.560 -0.178 1.00 30.10 ATOM 1158 N THR 1001 ATOM 1160 CA THR 1001 ATOM 1161 CB THR 1001

FIG. 7(23)

ATOM 1162 OG1 THR 1001 28.055 13.771 -0.605 1.00 33.54 ATOM 1164 CG2 THR 1001 25.878 12.741 -0.326 1.00 29.24 ATOM 1165 C THR 1001 29.303 12.388 1.338 1.00 27.68 ATOM 1166 O THR 1001 29.805 13.303 1.985 1.00 28.02 ATOM 1167 N LEU 1002 30.020 11.552 0.592 1.00 26.85 ATOM 1169 CA LEU 1002 31.454 11.636 0.572 1.00 24.39 ATOM 1170 CB LEU 1002 32.044 10.545 -0.298 1.00 22.71 ATOM 1171 CG LEU 1002 32.269 9.304 0.573 1.00 27.80 ATOM 1172 CD1 LEU 1002 32.727 8.142 -0.280 1.00 27.11 ATOM 1173 CD2 LEU 1002 33.295 9.592 1.670 1.00 24.64 ATOM 1174 C LEU 1002 31.908 12.995 0.099 1.00 26.97 ATOM 1175 O LEU 1002 32.967 13.459 0.506 1.00 26.84 ATOM 1176 N GLU 1003 31.063 13.682 -0.666 1.00 27.89 ATOM 1178 CA GLU 1003 31.428 15.000 -1.185 1.00 28.02 ATOM 1179 CB GLU 1003 30.419 15.503 -2.208 1.00 32.50 ATOM 1180 CG GLU 1003 30.988 16.624 -3.077 1.00 37.49 ATOM 1181 CD GLU 1003 31.915 16.121 -4.170 1.00 38.89 ATOM 1182 OE1 GLU 1003 33.065 15.743 -3.886 1.00 43.61 ATOM 1183 OE2 GLU 1003 31.488 16.102 -5.331 1.00 46.97 ATOM 1184 C GLU 1003 31.591 16.044 -0.117 1.00 25.24 ATOM 1185 O GLU 1003 32.485 16.885 -0.211 1.00 26.57 ATOM 1186 N HIS 1004 30.748 15.953 0.913 1.00 23.16 ATOM 1188 CA HIS 1004 30.746 16.884 2.040 1.00 19.58 ATOM 1189 CB HIS 1004 29.508 16.719 2.912 1.00 19.12 ATOM 1190 CG HIS 1004 28.227 17.024 2.208 1.00 23.47 ATOM 1191 CD2 HIS 1004 27.173 17.784 2.570 1.00 23.78 ATOM 1192 ND1 HIS 1004 27.911 16.508 0.964 1.00 27.88 26.718 16.936 0.596 1.00 20.57 ATOM 1194 CE1 HIS 1004 ATOM 1195 NE2 HIS 1004 26.246 17.710 1.554 1.00 23.61 ATOM 1197 C HIS 1004 31.940 16.631 2.885 1.00 21.64 ATOM 1198 O HIS 1004 32.753 17.508 3.075 1.00 25.00 ATOM 1199 N LEU 1005 32.055 15.419 3.394 1.00 23.11 ATOM 1201 CA LEU 1005 33.186 15.072 4.222 1.00 23.79 ATOM 1202 CB LEU 1005 33.131 13.581 4.589 1.00 24.17 ATOM 1203 CG LEU 1005 32.183 13.199 5.743 1.00 27.48 ATOM 1204 CD1 LEU 1005 31.030 14.150 5.821 1.00 25.44 ATOM 1205 CD2 LEU 1005 31.679 11.771 5.627 1.00 22.50 ATOM 1206 C LEU 1005 34.506 15.467 3.558 1.00 20.41 ATOM 1207 O LEU 1005 35.361 16.034 4.206 1.00 21.82 ATOM 1208 N ILE 1006 34.668 15.212 2.264 1.00 19.50

FIG. 7(24)

ATOM 1210 CA ILE 1006 35.914 15.589 1.609 1.00 18.77 36.128 14.806 0.276 1.00 16.46 37.602 14.777 -0.103 1.00 12.82 35.718 13.341 0.441 1.00 20 16 ATOM 1211 CB ILE 1006 ATOM 1212 CG2 ILE 1006 ATOM 1213 CG1 ILE 1006 35.718 13.341 0.441 1.00 20.16 ATOM 1214 CD1 ILE 1006 35.961 12.446 -0.834 1.00 11.88 ATOM 1215 C ILE 1006 35.998 17.136 1.377 1.00 22.88 37.11317.7301.4311.0021.2534.85417.7881.1081.0021.4734.86019.2400.9091.0021.6633.52219.8250.4311.0024.87 ATOM 1216 O ILE 1006 ATOM 1217 N CYS 1007 ATOM 1219 CA CYS 1007 ATOM 1220 CB CYS 1007 ATOM 1221 SG CYS 1007 33.760 21.544 -0.085 1.00 30.17 ATOM 1222 C CYS 1007 35.247 19.953 2.196 1.00 22.22 ATOM 1223 O CYS 1007 36.024 20.905 2.158 1.00 25.94 ATOM 1224 N TYR 1008 34.691 19.527 3.331 1.00 20.53 34.691 19.327 5.331 1.00 20.33 35.030 20.132 4.617 1.00 17.94 34.248 19.493 5.758 1.00 18.61 32.753 19.488 5.626 1.00 17.97 32.019 18.455 6.175 1.00 16.67 30.641 18.462 6.158 1.00 22.78 32.059 20.549 5.031 1.00 22.19 30.646 20.569 5.011 1.00 20.60 ATOM 1226 CA TYR 1008 ATOM 1227 CB TYR 1008 ATOM 1228 CG TYR 1008 ATOM 1229 CD1 TYR 1008 ATOM 1230 CE1 TYR 1008 ATOM 1231 CD2 TYR 1008 ATOM 1232 CE2 TYR 1008 29.949 19.513 5.579 1.00 23.22 28.574 19.454 5.551 1.00 18.30 36.537 19.945 4.883 1.00 18.55 ATOM 1233 CZ TYR 1008 ATOM 1234 OH TYR 1008 ATOM 1236 C TYR 1008 36.537 19.945 4.883 1.00 18.55 37.217 20.917 5.256 1.00 20.35 ATOM 1237 O TYR 1008 ATOM 1238 N SER 1009 37.056 18.726 4.642 1.00 14.74 ATOM 1240 CA SER 1009 38.476 18.409 4.852 1.00 13.39 ATOM 1241 CB SER 1009 38.810 16.962 4.473 1.00 17.24 ATOM 1242 OG SER 1009 38.018 16.001 5.152 1.00 26.04 ATOM 1244 C SER 1009 39.310 19.309 3.985 1.00 16.36 ATOM 1245 O SER 1009 40.317 19.864 4.446 1.00 20.21 38.953 19.375 2.699 1.00 20.97 39.654 20.246 1.742 1.00 23.34 38.985 20.126 0.365 1.00 18.83 39.605 21.002 -0.685 1.00 17.13 38.830 21.940 -1.370 1.00 13.94 40.979 20.918 -0.968 1.00 17.85 39.410 22.804 -2.339 1.00 16.30 ATOM 1246 N PHE 1010 ATOM 1248 CA PHE 1010 ATOM 1249 CB PHE 1010 ATOM 1250 CG PHE 1010 ATOM 1251 CD1 PHE 1010 ATOM 1252 CD2 PHE 1010 ATOM 1253 CE1 PHE 1010 41.569 21.763 -1.917 1.00 17.15 ATOM 1254 CE2 PHE 1010 40.772 22.714 -2.608 1.00 18.02 ATOM 1255 CZ PHE 1010

FIG. 7(25)

ATOM 1256 C PHE 1010 39.688 21.746 2.242 1.00 22.02

 39.688
 21.746
 2.242
 1.00 22.02

 40.749
 22.390
 2.298
 1.00 23.00

 38.535
 22.271
 2.643
 1.00 19.25

 38.418
 23.640
 3.159
 1.00 19.07

 36.980
 23.945
 3.480
 1.00 12.84

 36.117
 24.005
 2.270
 1.00 6.53

 34.713
 24.371
 2.659
 1.00 18.81

 34.490
 25.382
 3.347
 1.00 21.22

 33.760
 23.525
 2.302
 1.00 26.88

 39.262
 23.894
 4.394
 1.00 18.28

 39.840
 24.982
 4.543
 1.00 19.80

 39.270
 22.934
 5.319
 1.00 11.82

 40.110
 23.063
 6.500
 1.00 13.54

 39.825
 21.936
 7.528
 1.00 15.67

 40.686
 22.107
 8.795
 1.00 10.56

 38.370
 21.948
 7.901
 1.00 14.92

 41.618
 23.068
 6.068
 1.00 16.72

 ATOM 1257 O PHE 1010 ATOM 1258 N GLN 1011 ATOM 1260 CA GLN 1011 ATOM 1261 CB GLN 1011 ATOM 1262 CG GLN 1011 ATOM 1263 CD GLN 1011 ATOM 1264 OE1 GLN 1011 ATOM 1265 NE2 GLN 1011 ATOM 1268 C GLN 1011 ATOM 1269 O GLN 1011 ATOM 1270 N VAL 1012 ATOM 1272 CA VAL 1012 ATOM 1273 CB VAL 1012 ATOM 1274 CG1 VAL 1012 ATOM 1275 CG2 VAL 1012 41.618 23.068 6.068 1.00 16.72 42.448 23.782 6.665 1.00 20.48 ATOM 1276 C VAL 1012

 42.448
 23.782
 6.665
 1.00
 20.48

 42.001
 22.291
 5.051
 1.00
 15.90

 43.401
 22.352
 4.602
 1.00
 17.77

 43.732
 21.206
 3.638
 1.00
 10.59

 43.685
 23.755
 3.963
 1.00
 15.74

 44.764
 24.302
 4.139
 1.00
 17.49

 42.718
 24.342
 3.244
 1.00
 17.18

 42.866
 25.706
 2.665
 1.00
 15.11

 41.557
 26.152
 2.020
 1.00
 23.73

 41.146
 25.474
 0.748
 1.00
 23.57

 41.963
 26.033
 -0.354
 1.00
 26.38

 41.172
 25.978
 -1.617
 1.00
 38.71

 42.034
 26.404
 -2.776
 1.00
 50.36

 43.105
 26.678
 3.823
 1.00
 11.16

 44.066
 27.452
 3.818
 1.00
 13.85

 42.210
 26.590
 4.816
 1.00
 10.82

 42.250 ATOM 1277 O VAL 1012 ATOM 1278 N ALA 1013 ATOM 1280 CA ALA 1013 ATOM 1281 CB ALA 1013 ATOM 1282 C ALA 1013 ATOM 1283 O ALA 1013 ATOM 1284 N LYS 1014 ATOM 1286 CA LYS 1014 ATOM 1287 CB LYS 1014 ATOM 1288 CG LYS 1014 ATOM 1289 CD LYS 1014 ATOM 1290 CE LYS 1014 ATOM 1291 NZ LYS 1014 ATOM 1295 C LYS 1014 ATOM 1296 O LYS 1014 ATOM 1297 N GLY 1015 ATOM 1299 CA GLY 1015

 43.584
 27.327
 6.715
 1.00
 17.17

 44.124
 28.349
 7.130
 1.00
 19.92

 44.159
 26.128
 6.763
 1.00
 17.82

 45.426
 25.927
 7.439
 1.00
 15.78

 45.516
 24.488
 7.925
 1.00
 17.77

 44.538
 24.156
 9.057
 1.00
 15.19

 44.931
 24.991
 10.623
 1.00
 15.49

 ATOM 1300 C GLY 1015 ATOM 1301 O GLY 1015 ATOM 1302 N MET 1016 ATOM 1304 CA MET 1016 ATOM 1305 CB MET 1016 ATOM 1306 CG MET 1016 ATOM 1307 SD MET 1016

FIG. 7(26)

ATOM 1308 CE MET 1016 46.642 24.894 10.658 1.00 5.63 ATOM 1309 C MET 1016 46.625 26.321 6.618 1.00 14.62 ATOM 1310 O MET 1016 47.680 26.667 7.163 1.00 15.76 ATOM 1311 N GLU 1017 46.487 26.208 5.305 1.00 14.65 ATOM 1313 CA GLU 1017 47.552 26.608 4.384 1.00 21.43 ATOM 1314 CB GLU 1017 47.177 26.195 2.947 1.00 21.43 ATOM 1315 CG GLU 1017 48.162 26.622 1.878 1.00 22.82 ATOM 1316 CD GLU 1017 47.634 26.421 0.436 1.00 27.12 ATOM 1317 OE1 GLU 1017 46.457 26.769 0.141 1.00 24.95 ATOM 1318 OE2 GLU 1017 48.418 25.927 -0.424 1.00 32.93 ATOM 1319 C GLU 1017 47.667 28.145 4.535 1.00 18.38 ATOM 1320 O GLU 1017 48.760 28.668 4.593 1.00 17.43 46.526 28.839 4.677 1.00 19.09 46.509 30.295 4.894 1.00 20.74 ATOM 1321 N PHE 1018 ATOM 1323 CA PHE 1018 46.509 30.295 4.894 1.00 20.74 ATOM 1324 CB PHE 1018 45.067 30.848 4.870 1.00 27.18 44.942 32.338 5.248 1.00 25.91 44.477 32.718 6.521 1.00 26.19 ATOM 1325 CG PHE 1018 ATOM 1326 CD1 PHE 1018 ATOM 1327 CD2 PHE 1018 45.300 33.345 4.348 1.00 25.16 ATOM 1328 CE1 PHE 1018 44.381 34.059 6.890 1.00 27.10 ATOM 1329 CE2 PHE 1018 45.208 34.708 4.712 1.00 28.34 ATOM 1330 CZ PHE 1018 44.754 35.064 5.982 1.00 26.60 ATOM 1331 C PHE 1018 47.179 30.663 6.216 1.00 18.20 ATOM 1332 O PHE 1018 48.139 31.430 6.228 1.00 15.08 ATOM 1333 N LEU 1019 46.676 30.122 7.328 1.00 16.94 ATOM 1335 CA LEU 1019 47.259 30.414 8.654 1.00 19.44 ATOM 1336 CB LEU 1019 46.673 29.533 9.754 1.00 22.88 ATOM 1337 CG LEU 1019 45.238 29.773 10.165 1.00 24.41 ATOM 1338 CD1 LEU 1019 44.956 28.916 11.388 1.00 24.01 ATOM 1339 CD2 LEU 1019 45.084 31.277 10.485 1.00 25.61 ATOM 1340 C LEU 1019 48.736 30.173 8.660 1.00 19.44 ATOM 1341 O LEU 1019 49.493 30.896 9.316 1.00 18.98 ATOM 1342 N ALA 1020 49.135 29.076 8.023 1.00 19.45 ATOM 1344 CA ALA 1020 50.545 28.747 7.961 1.00 22.29 ATOM 1345 CB ALA 1020 50.748 27.350 7.397 1.00 21.86 ATOM 1346 C ALA 1020 51.252 29.829 7.115 1.00 26.13 ATOM 1347 O ALA 1020 52.348 30.257 7.471 1.00 25.25 ATOM 1348 N SER 1021 50.600 30.323 6.050 1.00 29.72 ATOM 1350 CA SER 1021 51.194 31.384 5.219 1.00 27.59 ATOM 1351 CB SER 1021 50.289 31.754 4.026 1.00 23.95

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FIG. 7(27)

ATOM 1352 OG SER 1021 49.252 32.662 4.349 1.00 22.60 ATOM 1354 C SER 1021 51.469 32.614 6.109 1.00 32.83

 51.469
 32.614
 6.109
 1.00
 32.83

 52.570
 33.172
 6.073
 1.00
 36.57

 50.513
 32.957
 6.981
 1.00
 31.88

 50.645
 34.093
 7.901
 1.00
 22.64

 49.294
 34.483
 8.465
 1.00
 17.89

 48.254
 34.691
 7.420
 1.00
 17.72

 48.648
 35.816
 6.468
 1.00
 18.00

 49.714
 36.666
 6.993
 1.00
 31.94

 49.625
 37.980
 7.168
 1.00
 30.72

 50.653
 38.644
 7.662
 1.00
 23.85

 48.508
 38.620
 6.862
 1.00
 40.00

 51.563
 33.787
 9.056
 1.00
 24.84

 ATOM 1355 O SER 1021 ATOM 1356 N ARG 1022 ATOM 1358 CA ARG 1022 ATOM 1359 CB ARG 1022 ATOM 1360 CG ARG 1022 ATOM 1361 CD ARG 1022 ATOM 1362 NE ARG 1022 ATOM 1364 CZ ARG 1022 ATOM 1365 NH1 ARG 1022 ATOM 1368 NH2 ARG 1022 51.563 33.787 9.056 1.00 24.84 51.718 34.612 9.960 1.00 23.27 52.115 32.576 9.061 1.00 23.84 53.039 32.137 10.094 1.00 23.59 54.237 33.067 10.196 1.00 22.44 52.404 31.899 11.456 1.00 25.21 53.054 32.024 12.504 1.00 28.54 ATOM 1371 C ARG 1022 ATOM 1372 O ARG 1022 ATOM 1373 N LYS 1023 ATOM 1375 CA LYS 1023 ATOM 1376 CB LYS 1023 ATOM 1377 C LYS 1023 53.054 32.024 12.504 1.00 28.54 51.164 31.435 11.411 1.00 20.82 50.404 31.114 12.595 1.00 28.12 48.982 31.709 12.472 1.00 30.32 48.936 33.504 12.847 1.00 33.73 50.388 29.576 12.720 1.00 30.32 ATOM 1378 O LYS 1023 ATOM 1379 N CYS 1024 ATOM 1381 CA CYS 1024 ATOM 1382 CB CYS 1024 ATOM 1383 SG CYS 1024

 50.388
 29.576
 12.729
 1.00
 32.20

 50.636
 28.882
 11.756
 1.00
 38.70

 50.167
 29.057
 13.934
 1.00
 30.55

 50.123
 27.619
 14.216
 1.00
 33.60

 51.406
 27.169
 14.970
 1.00
 36.10

 51.223
 25.807
 15.619
 1.00
 38.88

 52.585
 27.121
 13.988
 1.00
 38.38

 53.913
 27.422
 14.604
 1.00
 34.51

 48.891
 27.526
 15.104
 1.00
 33.66

 48.751
 28.301
 16.034
 1.00
 41.71

 47.958
 26.643
 14.797
 1.00
 31.27

 46.742
 26.570
 15.589
 1.00
 27.97

 45.691
 25.745
 14.861
 1.00
 23.43

 44.283
 26.091
 15.229
 1.00
 30.06

 43.342
 26.801
 14.560
 1.00
 33.43

 43.680
 25.659
 16.393
 1.00
 24.53

</table ATOM 1384 C CYS 1024 50.388 29.576 12.729 1.00 32.20 ATOM 1385 O CYS 1024 ATOM 1386 N ILE 1025 ATOM 1388 CA ILE 1025 ATOM 1389 CB ILE 1025 ATOM 1390 CG2 ILE 1025 ATOM 1391 CG1 ILE 1025 ATOM 1392 CD1 ILE 1025 ATOM 1393 C ILE 1025 ATOM 1394 O ILE 1025 ATOM 1395 N HIS 1026 ATOM 1397 CA HIS 1026 ATOM 1398 CB HIS 1026 ATOM 1399 CG HIS 1026 ATOM 1400 CD2 HIS 1026 ATOM 1401 ND1 HIS 1026

FIG. 7(28)

ATOM 1403 CE1 HIS 1026 42.428 26.085 16.424 1.00 26.31 ATOM 1404 NE2 HIS 1026 42.199 26.781 15.321 1.00 29.05 ATOM 1406 C HIS 1026 46.901 26.086 17.036 1.00 30.13 ATOM 1407 O HIS 1026 46.335 26.681 17.955 1.00 37.96 ATOM 1408 N ARG 1027 47.662 25.024 17.244 1.00 26.58 ATOM 1410 CA ARG 1027 47.872 24.429 18.583 1.00 31.87 ATOM 1411 CB ARG 1027 48.235 25.483 19.666 1.00 20.17 ATOM 1412 C ARG 1027 46.762 23.449 19.055 1.00 31.55 ATOM 1413 O ARG 1027 47.047 22.477 19.742 1.00 38.11 ATOM 1414 N ASP 1028 45.528 23.629 18.597 1.00 30.85 ATOM 1416 CA ASP 1028 44.466 22.698 18.955 1.00 26.34 ATOM 1417 CB ASP 1028 43.788 23.098 20.248 1.00 32.60 ATOM 1418 CG ASP 1028 42.847 22.020 20.755 1.00 35.64 ATOM 1419 OD1 ASP 1028 41.692 22.346 21.096 1.00 36.08 ATOM 1420 OD2 ASP 1028 43.267 20.842 20.790 1.00 40.39 ATOM 1421 C ASP 1028 43.435 22.565 17.841 1.00 26.23 ATOM 1422 O ASP 1028 42.276 22.926 17.998 1.00 23.40 ATOM 1423 N LEU 1029 43.884 22.034 16.708 1.00 24.88 ATOM 1425 CA LEU 1029 43.053 21.842 15.533 1.00 23.16 ATOM 1426 CB LEU 1029 43.958 21.772 14.299 1.00 18.78 ATOM 1427 CG LEU 1029 43.221 21.714 12.965 1.00 20.21 ATOM 1428 CD1 LEU 1029 42.349 22.952 12.812 1.00 15.13 ATOM 1429 CD2 LEU 1029 44.249 21.601 11.827 1.00 22.91 ATOM 1430 C LEU 1029 42.237 20.562 15.700 1.00 25.25 ATOM 1431 O LEU 1029 42.765 19.473 15.591 1.00 30.47 ATOM 1432 N ALA 1030 40.949 20.703 15.957 1.00 25.99 ATOM 1434 CA ALA 1030 40.062 19.574 16.182 1.00 25.19 ATOM 1435 CB ALA 1030 39.872 19.387 17.679 1.00 24.55 ATOM 1436 C ALA 1030 38.761 20.007 15.558 1.00 27.35 ATOM 1437 O ALA 1030 38.611 21.202 15.302 1.00 33.46 ATOM 1438 N ALA 1031 37.797 19.094 15.379 1.00 25.19 ATOM 1440 CA ALA 1031 36.508 19.451 14.752 1.00 22.16 ATOM 1441 CB ALA 1031 35.772 18.210 14.270 1.00 21.71 ATOM 1442 C ALA 1031 35.551 20.353 15.536 1.00 20.96 ATOM 1443 O ALA 1031 34.639 20.950 14.944 1.00 21.36 ATOM 1444 N ARG 1032 35.712 20.388 16.859 1.00 22.49 ATOM 1446 CA ARG 1032 34.898 21.246 17.736 1.00 27.01 ATOM 1447 CB ARG 1032 35.157 20.945 19.220 1.00 25.22 ATOM 1448 CG ARG 1032 36.534 21.451 19.707 1.00 34.44 ATOM 1449 CD ARG 1032 37.150 20.503 20.770 1.00 46.39

FIG. 7(29)

ATOM 1450 NE ARG 1032 38.554 20.752 21.158 1.00 41.28 ATOM 1452 CZ ARG 1032 39.464 19.799 21.352 1.00 32.28 ATOM 1453 NH1 ARG 1032 40.677 20.129 21.709 1.00 27.74 ATOM 1456 NH2 ARG 1032 39.178 18.524 21.148 1.00 31.24 ATOM 1459 C ARG 1032 35.296 22.708 17.482 1.00 25.91 34.601 23.605 17.935 1.00 30.23 ATOM 1460 O ARG 1032 ATOM 1461 N ASN 1033 36.451 22.911 16.840 1.00 20.90 ATOM 1463 CA ASN 1033 37.008 24.222 16.495 1.00 15.77 ATOM 1464 CB ASN 1033 38.497 24.290 16.813 1.00 18.29 ATOM 1465 CG ASN 1033 38.760 24.160 18.254 1.00 20.60 ATOM 1466 OD1 ASN 1033 37.891 24.445 19.067 1.00 29.84 ATOM 1467 ND2 ASN 1033 39.929 23.677 18.601 1.00 18.08 ATOM 1470 C ASN 1033 36.839 24.535 15.019 1.00 19.29 ATOM 1471 O ASN 1033 37.619 25.303 14.450 1.00 17.18 ATOM 1472 N ILE 1034 35.934 23.822 14.366 1.00 17.56 ATOM 1474 CA ILE 1034 35.631 24.092 12.972 1.00 17.92 ATOM 1475 CB ILE 1034 35.813 22.868 12.091 1.00 15.66 ATOM 1476 CG2 ILE 1034 35.364 23.192 10.647 1.00 12.61 ATOM 1477 CG1 ILE 1034 37.247 22.349 12.221 1.00 10.08 ATOM 1478 CD1 ILE 1034 38.312 23.384 11.994 1.00 18.10 ATOM 1479 C ILE 1034 34.147 24.381 13.075 1.00 21.87 ATOM 1480 O ILE 1034 33.410 23.592 13.669 1.00 26.72 ATOM 1481 N LEU 1035 33.711 25.524 12.575 1.00 21.91 ATOM 1483 CA LEU 1035 32.311 25.883 12.670 1.00 19.45 ATOM 1484 CB LEU 1035 32.190 27.310 13.181 1.00 18.73 ATOM 1485 CG LEU 1035 32.102 27.454 14.691 1.00 21.53 ATOM 1486 CD1 LEU 1035 33.019 26.518 15.456 1.00 8.66 ATOM 1487 CD2 LEU 1035 32.391 28.881 15.016 1.00 19.34 ATOM 1488 C LEU 1035 31.700 25.764 11.316 1.00 20.15 ATOM 1489 O LEU 1035 32.377 25.977 10.310 1.00 21.51 ATOM 1490 N LEU 1036 30.429 25.390 11.275 1.00 24.13 ATOM 1492 CA LEU 1036 29.745 25.237 10.006 1.00 26.96 ATOM 1493 CB LEU 1036 29.027 23.882 9.909 1.00 20.57 28.149 23.631 8.081 1.00 1.23 28.877 23.617 7.360 1.00 7.53 27.566 22.306 8.900 1.00 18.85 ATOM 1494 CG LEU 1036 28.149 23.631 8.681 1.00 17.23

 20.077
 23.617
 7.360
 1.00
 7.53

 27.566
 22.306
 8.900
 1.00
 18.85

 28.827
 26.432
 9.755
 1.00
 31.45

 27.953
 26.794
 10.557
 1.00
 29.93

 29.094
 27.061
 8.628
 1.00
 34.52

 28.410
 28.248
 8.215
 1.00
 37.27

 ATOM 1495 CD1 LEU 1036 ATOM 1496 CD2 LEU 1036 ATOM 1497 C LEU 1036 ATOM 1498 O LEU-1036 ATOM 1499 N SER 1037 ATOM 1501 CA SER 1037

FIG. 7(30)

ATOM 1502 CB SER 1037 29.448 29.220 7.632 1.00 41.11 ATOM 1503 OG SER 1037 28.879 30.439 7.193 1.00 44.80 ATOM 1505 C SER 1037 27.367 27.890 7.209 1.00 39.39 ATOM 1506 O SER 1037 27.045 26.735 7.024 1.00 42.14 ATOM 1507 N GLU 1038 26.884 28.912 6.531 1.00 44.94 ATOM 1509 CA GLU 1038 25.845 28.806 5.534 1.00 50.37 ATOM 1510 CB GLU 1038 25.685 30.152 4.792 1.00 56.15 ATOM 1511 CG GLU 1038 25.599 31.391 5.676 1.00 55.19 ATOM 1512 CD GLU 1038 24.518 31.270 6.708 1.00 59.42 ATOM 1513 OE1 GLU 1038 23.464 30.637 6.419 1.00 58.62 ATOM 1514 OE2 GLU 1038 24.736 31.806 7.816 1.00 63.52 ATOM 1515 C GLU 1038 25.954 27.672 4.518 1.00 51.35 ATOM 1516 O GLU 1038 25.619 26.521 4.816 1.00 57.04 ATOM 1517 N LYS 1039 26.414 27.997 3.317 1.00 46.28 ATOM 1519 CA LYS 1039 26.467 27.021 2.251 1.00 43.05 ATOM 1520 CB LYS 1039 26.455 27.729 0.898 1.00 41.05 ATOM 1521 C LYS 1039 27.689 26.155 2.401 1.00 44.31 ATOM 1522 O LYS 1039 28.687 26.358 1.697 1.00 50.06 ATOM 1523 N ASN 1040 27.611 25.210 3.339 1.00 37.02 ATOM 1525 CA ASN 1040 28.701 24.283 3.630 1.00 32.65 ATOM 1526 CB ASN 1040 28.647 23.041 2.761 1.00 31.69 ATOM 1527 CG ASN 1040 27.641 22.061 3.267 1.00 31.29 ATOM 1528 OD1 ASN 1040 26.740 21.693 2.553 1.00 38.80 ATOM 1529 ND2 ASN 1040 27.749 21.680 4.530 1.00 36.05 ATOM 1532 C ASN 1040 30.096 24.844 3.656 1.00 28.45 ATOM 1533 O ASN 1040 31.079 24.162 3.300 1.00 26.00 ATOM 1534 N VAL 1041 30.174 26.101 4.073 1.00 23.77 ATOM 1536 CA VAL 1041 31.447 26.739 4.207 1.00 16.56 ATOM 1537 CB VAL 1041 31.382 28.274 3.940 1.00 16.16 ATOM 1538 CG1 VAL 1041 32.709 28.948 4.315 1.00 8.57 ATOM 1539 CG2 VAL 1041 31.124 28.509 2.470 1.00 6.79 ATOM 1540 C VAL 1041 31.726 26.382 5.646 1.00 15.50 ATOM 1541 O VAL 1041 30.825 26.333 6.485 1.00 9.73 ATOM 1542 N VAL 1042 32,967 26,022 5,883 1,00 18,82 ATOM 1544 CA VAL 1042 33.431 25.607 7.185 1.00 19.76 ATOM 1545 CB VAL 1042 33.907 24.110 7.051 1.00 22.19 ATOM 1546 CG1 VAL 1042 35.439 23.993 7.041 1.00 18.66 ATOM 1547 CG2 VAL 1042 33.247 23.242 8.100 1.00 22.95 ATOM 1548 C VAL 1042 34.580 26.607 7.483 1.00 20.50 ATOM 1549 O VAL 1042 35.348 26.960 6.575 1.00 17.75

FIG. 7(31)

ATOM 1550 N LYS 1043 34.675 27.082 8.726 1.00 18.30 ATOM 1552 CA LYS 1043 35.679 28.070 9.103 1.00 17.43 ATOM 1553 CB LYS 1043 34.977 29.420 9.277 1.00 17.68 ATOM 1554 CG LYS 1043 34.202 29.845 8.031 1.00 19.19 ATOM 1555 CD LYS 1043 33.560 31.228 8.186 1.00 26.86 ATOM 1556 CE LYS 1043 33.270 31.885 6.820 1.00 18.32 ATOM 1557 NZ LYS 1043 34.353 32.806 6.425 1.00 22.63 ATOM 1561 C LYS 1043 36.373 27.687 10.399 1.00 18.35 ATOM 1562 O LYS 1043 35.709 27.235 11.330 1.00 17.37 ATOM 1563 N ILE 1044 37.692 27.880 10.461 1.00 17.47 ATOM 1565 CA ILE 1044 38.504 27.558 11.645 1.00 21.49 ATOM 1566 CB ILE 1044 40.010 27.390 11.267 1.00 20.48 ATOM 1567 CG2 ILE 1044 40.896 27.250 12.502 1.00 15.75 ATOM 1568 CG1 ILE 1044 40.221 26.237 10.300 1.00 14.66 41.584 26.344 9.669 1.00 12.76 ATOM 1569 CD1 ILE 1044 ATOM 1570 C ILE 1044 38.432 28.735 12.626 1.00 30.73 ATOM 1571 O ILE 1044 38.370 29.888 12.207 1.00 31.68 ATOM 1572 N CYS 1045 38.454 28.436 13.918 1.00 38.50 ATOM 1574 CA-CYS 1045 38.437 29.444 14.968 1.00 48.73 ATOM 1575 CB CYS 1045 37.027 29.586 15.558 1.00 50.35 ATOM 1576 SG CYS 1045 36.259 28.069 16.173 1.00 59.69 ATOM 1577 C CYS 1045 39.473 29.041 16.033 1.00 54.63 ATOM 1578 O CYS 1045 39.981 27.912 15.986 1.00 54.88 ATOM 1579 N ASP 1046 39.811 29.954 16.956 1.00 64.20 ATOM 1581 CA ASP 1046 40.816 29.700 18.021 1.00 69.98 ATOM 1582 CB ASP 1046 40.454 28.407 18.788 1.00 72.94 ATOM 1583 CG ASP 1046 41.338 28.165 20.009 1.00 75.40 ATOM 1584 OD1 ASP 1046 40.930 28.584 21.110 1.00 77.66 ATOM 1585 OD2 ASP 1046 42.428 27.547 19.878 1.00 75.18 ATOM 1586 C ASP 1046 42.219 29.580 17.354 1.00 74.21 ATOM 1587 O ASP 1046 43.183 29.036 17.940 1.00 74.94 ATOM 1588 N PHE 1047 42.307 30.205 16.171 1.00 75.46 ATOM 1590 CA PHE 1047 43.462 30.212 15.245 1.00 71.53 ATOM 1591 CB PHE 1047 42.919 30.267 13.790 1.00 72.10 ATOM 1592 CG PHE 1047 41.906 31.381 13.526 1.00 71.34 ATOM 1593 CD1 PHE 1047 42.139 32.327 12.526 1.00 74.26 ATOM 1594 CD2 PHE 1047 40.747 31.501 14.284 1.00 69.46 ATOM 1595 CE1 PHE 1047 41.242 33.367 12.293 1.00 70.87 ATOM 1596 CE2 PHE 1047 39.847 32.533 14.066 1.00 67.97 ATOM 1597 CZ PHE 1047 40.096 33.467 13.068 1.00 71.41

FIG. 7(32)

ATOM 1598 C PHE 1047 44.681 31.163 15.426 1.00 67.78 ATOM 1599 O PHE 1047 44.507 32.345 15.797 1.00 63.26 ATOM 1601 CB ASP 1064 29.579 17.003 25.123 1.00 69.86 ATOM 1602 CG ASP 1064 30.534 16.464 24.050 1.00 69.93 ATOM 1603 OD1 ASP 1064 31.028 15.321 24.179 1.00 71.35 ATOM 1604 OD2 ASP 1064 30.776 17.189 23.063 1.00 71.45 ATOM 1605 C ASP 1064 31.511 17.821 26.539 1.00 64.90 ATOM 1606 O ASP 1064 31.512 19.029 26.788 1.00 64.09 ATOM 1609 N ASP 1064 29.229 17.550 27.534 1.00 67.30 ATOM 1611 CA ASP 1064 30.204 17.019 26.533 1.00 67.58 ATOM 1612 N ALA 1065 32.617 17.135 26.278 1.00 61.87 ATOM 1614 CA ALA 1065 33.932 17.759 26.244 1.00 58.06 ATOM 1615 CB ALA 1065 34.479 17.935 27.650 1.00 56.61 ATOM 1616 C ALA 1065 34.888 16.915 25.397 1.00 57.97 34.491 15.906 24.788 1.00 56.86 ATOM 1617 O ALA 1065 ATOM 1618 N ARG 1066 36.155 17.313 25.400 1.00 54.64 ATOM 1620 CA ARG 1066 37.182 16.664 24.607 1.00 50.99 ATOM 1621 CB ARG 1066 37.538 17.539 23.393 1.00 49.53 ATOM 1622 CG ARG 1066 36.459 17.608 22.335 1.00 52.76 ATOM 1623 CD ARG 1066 36.866 16.805 21.125 1.00 57.63 ATOM 1624 NE ARG 1066 35.847 16.645 20.093 1.00 57.02 ATOM 1626 CZ ARG 1066 35.976 17.033 18.824 1.00 55.63 1627 NH1 ARG 1066 MOTA 34.984 16.797 17.995 1.00 57.63 ATOM 1630 NH2 ARG 1066 37.046 17.691 18.385 1.00 40.52 ATOM 1633 C ARG 1066 38.428 16.513 25.427 1.00 49.01 ATOM 1634 O ARG 1066 38.652 17.274 26.364 1.00 46.29 ATOM 1635 N LEU 1067 39.251 15.546 25.041 1.00 46.48 ATOM 1637 CA LEU 1067 40.510 15.320 25.709 1.00 45.62 ATOM 1638 CB LEU 1067 40.703 13.840 26.073 1.00 45.53 MOTA 1639 CG LEU 1067 41.335 13.519 27.441 1.00 44.07 ATOM 1640 CD1 LEU 1067 42.236 12.322 27.273 1.00 37.52 ATOM 1641 CD2 LEU 1067 42.109 14.710 28.057 1.00 39.60 ATOM 1642 C LEU 1067 41.530 15.778 24.677 1.00 42.00 41.983 15.010 23.832 1.00 41.05 ATOM 1643 O LEU 1067 ATOM 1644 N PRO 1068 41.854 17.072 24.698 1.00 41.22 41.265 18.104 25.584 1.00 34.16 42.817 17.661 23.761 1.00 38.41 42.919 19.104 24.277 1.00 36.08 41.496 19.355 24.828 1.00 29.23 ATOM 1645 CD PRO 1068 ATOM 1646 CA PRO 1068 ATOM ·1647 CB PRO 1068 ATOM 1648 CG PRO 1068 ATOM 1649 C PRO 1068 44.197 16.961 23.571 1.00 35.36

FIG. 7(33)

ATOM 1650 O PRO 1068 44.932 17.258 22.623 1.00 37.80 ATOM 1651 N LEU 1069 44.552 16.040 24.455 1.00 33.98 ATOM 1653 CA LEU 1069 45.829 15.337 24.333 1.00 35.06 ATOM 1654 CB LEU 1069 46.092 14.517 25.601 1.00 37.80 ATOM 1655 CG LEU 1069 47.228 13.497 25.488 1.00 40.67 ATOM 1656 CD1 LEU 1069 48.599 14.156 25.752 1.00 36.35 ATOM 1657 CD2 LEU 1069 46.939 12.333 26.445 1.00 40.75 ATOM 1658 C LEU 1069 45.776 14.397 23.121 1.00 34.16 ATOM 1659 O LEU 1069 46.787 14.115 22.461 1.00 32.14 ATOM 1660 N LYS 1070 44.571 13.916 22.859 1.00 28.95 ATOM 1662 CA LYS 1070 44.280 13.014 21.765 1.00 28.17 ATOM 1663 CB LYS 1070 42.828 12.569 21.911 1.00 22.17 ATOM 1664 CG LYS 1070 42.553 11.730 23.144 1.00 22.02 ATOM 1665 CD LYS 1070 41.085 11.317 23.107 1.00 24.17 ATOM 1666 CE LYS 1070 40.851 9.908 23.646 1.00 29.35 ATOM 1667 NZ LYS 1070 39.444 9.436 23.439 1.00 35.82 ATOM 1671 C LYS 1070 44.518 13.582 20.340 1.00 29.26 ATOM 1672 O LYS 1070 44.368 12.867 19.344 1.00 27.81 ATOM 1673 N TRP 1071 44.862 14.865 20.260 1.00 27.00 ATOM 1675 CA TRP 1071 45.086 15.550 18.995 1.00 27.37 ATOM 1676 CB TRP 1071 44.191 16.827 18.882 1.00 20.67 ATOM 1677 CG TRP 1071 42.724 16.551 18.545 1.00 20.12 ATOM 1678 CD2 TRP 1071 41.685 16.138 19.451 1.00 17.97 ATOM 1679 CE2 TRP 1071 40.524 15.892 18.675 1.00 13.02 ATOM 1680 CE3 TRP 1071 41.628 15.944 20.838 1.00 23.76 ATOM 1681 CD1 TRP 1071 42.153 16.560 17.304 1.00 19.50 ATOM 1682 NE1 TRP 1071 40.834 16.155 17.373 1.00 13.62 ATOM 1684 CZ2 TRP 1071 39.342 15.465 19.233 1.00 16.22 ATOM 1685 CZ3 TRP 1071 40.439 15.511 21.396 1.00 20.67 ATOM 1686 CH2 TRP 1071 39.321 15.273 20.594 1.00 19.47 ATOM 1687 C TRP 1071 46.523 15.961 18.889 1.00 26.26 ATOM 1688 O TRP 1071 46.948 16.465 17.842 1.00 28.70 ATOM 1689 N MET 1072 47.278 15.713 19.959 1.00 24.85 ATOM 1691 CA MET 1072 48.676 16.119 20.034 1.00 22.67 ATOM 1692 CB MET 1072 49.066 16.317 21.487 1.00 31.30 ATOM 1693 CG MET 1072 48.328 17.416 22.229 1.00 34.64 ATOM 1694 SD MET 1072 48.977 17.610 23.948 1.00 35.65 ATOM 1695 CE MET 1072 50.667 17.842 23.669 1.00 27.97 ATOM 1696 C MET 1072 49.697 15.215 19.388 1.00 25.43 ATOM 1697 O MET 1072 49.798 14.029 19.729 1.00 21.51

FIG. 7(34)

ATOM 1698 N ALA 1073 50.545 15.800 18.547 1.00 25.55 ATOM 1700 CA ALA 1073 51.571 15.024 17.874 1.00 29.80 ATOM 1701 CB ALA 1073 52.369 15.912 16.958 1.00 22.65 ATOM 1702 C ALA 1073 52.448 14.453 18.989 1.00 34.88 ATOM 1703 O ALA 1073 52.431 14.970 20.115 1.00 39.38 53.183 13.355 18.724 1.00 36.01 53.087 12.450 17.570 1.00 31.55 54.040 12.771 19.769 1.00 36.24 ATOM 1704 N PRO 1074 ATOM 1705 CD PRO 1074 ATOM: 1706 CA PRO 1074 ATOM 1707 CB PRO 1074 54.544 11.485 19.115 1.00 34.34 ATOM 1708 CG PRO 1074 53.415 11.137 18.193 1.00 31.88

 55.189
 13.670
 20.288
 1.00 37.13

 55.570
 13.575
 21.447
 1.00 34.58

 55.746
 14.533
 19.440
 1.00 37.40

 56.813
 15.422
 19.884
 1.00 40.62

 57.598
 15.990
 18.707
 1.00 33.55

 56.853
 16.957
 17.844
 1.00 39.40

 55.952
 16.300
 16.828
 1.00 43.14

 55.965
 15.055
 16.720
 1.00 49.09

 55.228
 17.040
 16.124
 1.00 44.63

 ATOM 1709 C PRO 1074 55.189 13.670 20.288 1.00 37.13 ATOM 1710 O PRO 1074 ATOM 1711 N GLU 1075 ATOM 1713 CA GLU 1075 ATOM 1714 CB GLU 1075 ATOM 1715 CG GLU 1075 ATOM 1716 CD GLU 1075 ATOM 1717 OE1 GLU 1075 ATOM 1718 OE2 GLU 1075 55.228 17.040 16.124 1.00 44.63 ATOM 1719 C GLU 1075 56.239 16.546 20.757 1.00 42.73 ATOM 1720 O GLU 1075 56.903 17.061 21.639 1.00 44.76 ATOM 1721 N THR 1076 54.982 16.888 20.524 1.00 46.13 ATOM 1723 CA THR 1076 54.304 17.923 21.283 1.00 46.22 52.991 18.319 20.605 1.00 43.95 ATOM 1724 CB THR 1076 ATOM 1725 OG1 THR 1076 53.245 18.666 19.230 1.00 46.46 ATOM 1727 CG2 THR 1076 52.361 19.481 21.334 1.00 43.93 ATOM 1728 C THR 1076 53.991 17.378 22.662 1.00 47.62 ATOM 1729 O THR 1076 54.175 18.057 23.650 1.00 52.45 53.442 16.173 22.717 1.00 47.96 53.123 15.528 23.980 1.00 46.99 52.496 14.151 23.720 1.00 46.43 52.691 13.232 24.895 1.00 46.16 51.024 14.306 23.384 1.00 44.29 ATOM 1730 N ILE 1077 53.442 16.173 22.717 1.00 47.96 ATOM 1732 CA ILE 1077 ATOM 1733 CB ILE 1077 ATOM 1734 CG2 ILE 1077 ATOM 1735 CG1 ILE 1077 ATOM 1736 CD1 ILE 1077 50.336 13.010 23.163 1.00 46.43 ATOM 1737 C ILE 1077 54.418 15.345 24.767 1.00 51.37 54.473 15.577 25.974 1.00 52.53 55.458 14.931 24.058 1.00 53.41 56.750 14.696 24.672 1.00 58.94 57.506 13.570 23.925 1.00 60.74 ATOM 1738 O ILE 1077 ATOM 1739 N PHE 1078 ATOM 1741 CA PHE 1078 ATOM 1742 CB PHE 1078 ATOM 1743 CG PHE 1078 56.901 12.184 24.124 1.00 57.84

FIG. 7(35)

ATOM 1744 CD1 PHE 1078 56.068 11.612 23.169 1.00 54.09 ATOM 1745 CD2 PHE 1078 57.127 11.483 25.298 1.00 58.64 ATOM 1746 CE1 PHE 1078 55.478 10.380 23.381 1.00 53.82 56.539 10.254 25.514 1.00 57.20 ATOM 1747 CE2 PHE 1078 ATOM 1748 CZ PHE 1078 55.711 9.703 24.555 1.00 55.07 ATOM 1749 C PHE 1078 57.574 15.981 24.767 1.00 63.98 ATOM 1750 O PHE 1078 57.433 16.738 25.736 1.00 67.06 ATOM 1751 N ASP 1079 58.356 16.274 23.724 1.00 66.97 59.215 17.472 23.678 1.00 68.09 ATOM 1753 CA ASP 1079 ATOM 1754 CB ASP 1079 60.225 17.402 22.501 1.00 66.89 ATOM 1755 CG ASP 1079 60.174 16.082 21.714 1.00 69.02 ATOM 1756 OD1 ASP 1079 60.254 16.156 20.474 1.00 71.23 ATOM 1757 OD2 ASP 1079 60.089 14.980 22.308 1.00 69.71 ATOM 1758 C ASP 1079 58.434 18.806 23.599 1.00 67.74 59.011 19.848 23.266 1.00 66.85 ATOM 1759 O ASP 1079 ATOM 1760 N ARG 1080 57.137 18.747 23.926 1.00 68.20 ATOM 1762 CA ARG 1080 56.173 19.858 23.898 1.00 66.60 ATOM 1763 CB ARG 1080 55.997 20.496 25.279 1.00 67.64 ATOM 1764 CG ARG 1080 54.529 20.758 25.638 1.00 71.26 ATOM 1765 CD ARG 1080 53.823 19.481 26.096 1.00 73.66 ATOM 1766 NE ARG 1080 52.364 19.610 26.226 1.00 75.75 ATOM 1768 CZ ARG 1080 51.642 18.981 27.157 1.00 74.86 ATOM 1769 NH1 ARG 1080 50.321 19.134 27.211 1.00 69.96 ATOM 1772 NH2 ARG 1080 52.247 18.212 28.060 1.00 72.78 ATOM 1775 C ARG 1080 56.305 20.920 22.801 1.00 63.93 ATOM 1776 O ARG 1080 55.861 22.069 22.955 1.00 61.93 56.863 20.510 21.667 1.00 61.30 ATOM 1777 N VAL 1081 ATOM 1779 CA VAL 1081 57.034 21.413 20.545 1.00 58.53 ATOM 1780 CB VAL 1081 58.202 20.951 19.584 1.00 60.54 ATOM 1781 CG1 VAL 1081 59.304 20.266 20.370 1.00 62.35 ATOM 1782 CG2 VAL 1081 57.701 20.043 18.455 1.00 55.04 55.713 21.481 19.771 1.00 56.90 ATOM 1783 C VAL 1081 ATOM 1784 O VAL 1081 55.052 20.452 19.560 1.00 57.43 ATOM 1785 N TYR 1082 55.287 22.699 19.435 1.00 51.51 ATOM 1787 CA TYR 1082 54.078 22.909 18.641 1.00 41.08 ATOM 1788 CB TYR 1082 53.092 23.847 19.332 1.00 37.59 ATOM 1789 CG TYR 1082 52.275 23.238 20.442 1.00 32.41 ATOM 1790 CD1 TYR 1082 52.800 23.135 21.721 1.00 38.13 ATOM 1791 CE1 TYR 1082 52.043 22.663 22.781 1.00 38.73 ATOM 1792 CD2 TYR 1082 50.961 22.843 20.234 1.00 27.91

FIG. 7(36)

50.189 22.374 21.287 1.00 33.59 ATOM 1793 CE2 TYR 1082 50.739 22.290 22.572 1.00 36.82 ATOM 1794 CZ TYR 1082 ATOM 1795 OH TYR 1082 50.001 21.874 23.679 1.00 39.60 54.591 23.598 17.410 1.00 34.81 ATOM 1797 C TYR 1082 55.240 24.608 17.545 1.00 33.62 ATOM 1798 O TYR 1082 54.394 22.997 16.236 1.00 34.71 ATOM 1799 N THR 1083 54.819 23.573 14.946 1.00 30.90 ATOM 1801 CA THR 1083 56.106 22.894 14.384 1.00 29.46 ATOM 1802 CB THR 1083 55.789 21.598 13.837 1.00 30.18 ATOM 1803 OG1 THR 1083 57.159 22.768 15.486 1.00 21.74 ATOM 1805 CG2 THR 1083 53.678 23.371 13.946 1.00 27.79 ATOM 1806 C THR 1083 52.651 22.777 14.293 1.00 28.80 ATOM 1807 O THR 1083 53.804 23.869 12.721 1.00 24.37 ATOM 1808 N ILE 1084 52.700 23.615 11.797 1.00 27.69 ATOM 1810 CA ILE 1084 52.739 24.381 10.465 1.00 28.65 ATOM 1811 CB ILE 1084 51.450 25.166 10.284 1.00 29.19 ATOM 1812 CG2 ILE 1084 53.977 25.259 10.361 1.00 37.75 ATOM 1813 CG1 ILE 1084 55.235 24.517 9.985 1.00 46.61 ATOM 1814 CD1 ILE 1084 ATOM 1815 C ILE 1084 52.689 22.143 11.459 1.00 26.44 51.627 21.589 11.173 1.00 24.29 ATOM 1816 O ILE 1084 53.861 21.507 11.518 1.00 25.11 ATOM 1817 N GLN 1085 53.920 20.097 11.188 1.00 24.39 ATOM 1819 CA GLN 1085 55.315 19.612 10.823 1.00 27.61 ATOM 1820 CB GLN 1085 55.753 20.012 9.411 1.00 33.25 ATOM 1821 CG GLN 1085 ATOM 1822 CD GLN 1085 54.653 19.826 8.347 1.00 34.07 53.943 20.779 8.004 1.00 41.60 ATOM 1823 OE1 GLN 1085 54.546 18.632 7.797 1.00 28.88 ATOM 1824 NE2 GLN 1085 53.296 19.267 12.258 1.00 23.23 ATOM 1827 C GLN 1085 52.900 18.141 11.981 1.00 25.97 ATOM 1828 O GLN 1085 53.195 19.798 13.480 1.00 20.86 ATOM 1829 N SER 1086 52.488 19.040 14.507 1.00 18.08 ATOM 1831 CA SER 1086 ATOM 1832 CB SER 1086 53.044 19.256 15.926 1.00 20.91 52.870 20.559 16.440 1.00 21.60 ATOM 1833 OG SER 1086 ATOM 1835 C SER 1086 50.962 19.336 14.353 1.00 20.67 50.138 18.531 14.806 1.00 13.79 ATOM 1836 O SER 1086 50.602 20.415 13.609 1.00 18.68 ATOM 1837 N ASP 1087 49.190 20.793 13.324 1.00 11.08 ATOM 1839 CA ASP 1087 49.038 22.249 12.805 1.00 21.08 ATOM 1840 CB ASP 1087 48.845 23.287 13.920 1.00 23.79 ATOM 1841 CG ASP 1087 49.348 24.407 13.745 1.00 31.01 ATOM 1842 OD1 ASP 1087

FIG. 7(37)

48.212 23.013 14.967 1.00 28.91 ATOM 1843 OD2 ASP 1087 48.632 19.860 12.261 1.00 11.16 ATOM 1844 C ASP 1087 47.406 19.640 12.177 1.00 12.65 ATOM 1845 O ASP 1087 49.520 19.390 11.390 1.00 9.61 ATOM 1846 N VAL 1088 49.181 18.404 10.345 1.00 13.37 ATOM 1848 CA VAL 1088 50.351 18.195 9.389 1.00 15.40 ATOM 1849 CB VAL 1088 ATOM 1850 CG1 VAL 1088 50.057 17.067 8.486 1.00 14.68 50.609 19.477 8.587 1.00 10.67 ATOM 1851 CG2 VAL 1088 48.839 17.061 11.014 1.00 13.67 ATOM 1852 C VAL 1088 47.897 16.387 10.618 1.00 15.00 ATOM 1853 O VAL 1088 49.618 16.668 12.015 1.00 12.30 ATOM 1854 N TRP 1089 ATOM 1856 CA TRP 1089 49.301 15.460 12.748 1.00 12.96 50.236 15.279 13.960 1.00 16.98 ATOM 1857 CB TRP 1089 49.764 14.195 14.887 1.00 18.14 ATOM 1858 CG TRP 1089 50.325 12.884 15.031 1.00 18.48 ATOM 1859 CD2 TRP 1089 49.476 12.162 15.893 1.00 20.05 ATOM 1860 CE2 TRP 1089 51.460 12.245 14.503 1.00 22.61 ATOM 1861 CE3 TRP 1089 48.640 14.215 15.657 1.00 18.89 ATOM 1862 CD1 TRP 1089 48.451 12.995 16.255 1.00 19.54 ATOM 1863 NE1 TRP 1089 49.725 10.839 16.249 1.00 20.08 ATOM 1865 CZ2 TRP 1089 51.709 10.927 14.855 1.00 17.00 ATOM 1866 CZ3 TRP 1089 50.846 10.243 15.722 1.00 23.71 ATOM 1867 CH2 TRP 1089 47.873 15.711 13.207 1.00 14.68 ATOM 1868 C TRP 1089 46.987 14.958 12.842 1.00 20.33 ATOM 1869 O TRP 1089 47.636 16.823 13.923 1.00 18.59 ATOM 1870 N SER 1090 46.287 17.209 14.413 1.00 15.54 ATOM 1872 CA SER 1090 46.297 18.603 15.043 1.00 12.20 ATOM 1873 CB SER 1090 47.066 18.621 16.237 1.00 18.86 ATOM 1874 OG SER 1090 45.256 17.190 13.309 1.00 16.50 ATOM 1876 C SER 1090 ATOM 1877 O SER 1090 44.128 16.691 13.487 1.00 18.14 ATOM 1878 N PHE 1091 45.635 17.745 12.158 1.00 23.35 44.746 17.776 10.997 1.00 20.78 ATOM 1880 CA PHE 1091 45.445 18.399 9.786 1.00 17.07 ATOM 1881 CB PHE 1091 44.533 18.524 8.598 1.00 21.98 ATOM 1882 CG PHE 1091 43.396 19.347 8.666 1.00 17.34 ATOM 1883 CD1 PHE 1091 44.740 17.754 7.460 1.00 19.42 ATOM 1884 CD2 PHE 1091 42.485 19.398 7.641 1.00 15.43 ATOM 1885 CE1 PHE 1091 43.829 17.792 6.421 1.00 18.06 ATOM 1886 CE2 PHE 1091 42.693 18.618 6.509 1.00 19.76 ATOM 1887 CZ PHE 1091 44.306 16.332 10.667 1.00 17.25 ATOM 1888 C PHE 1091

FIG. 7(38)

ATOM 1889 O PHE 1091 43.147 16.077 10.334 1.00 15.79 45.258 15.408 10.812 1.00 19.49 ATOM 1890 N GLY 1092 45.042 13.988 10.577 1.00 18.11 ATOM 1892 CA GLY 1092 44.029 13.429 11.544 1.00 19.35 ATOM 1893 C GLY 1092 43.235 12.581 11.137 1.00 24.23 ATOM 1894 O GLY 1092 44.073 13.836 12.819 1.00 18.53 ATOM 1895 N VAL 1093 43.055 13.392 13.788 1.00 20.09 ATOM 1897 CA VAL 1093 43.389 13.752 15.298 1.00 15.18 ATOM 1898 CB VAL 1093 42.421 13.051 16.187 1.00 17.08 ATOM 1899 CG1 VAL 1093 44.778 13.310 15.698 1.00 11.27 ATOM 1900 CG2 VAL 1093 41.661 13.971 13.376 1.00 22.42 ATOM 1901 C VAL 1093 40.649 13.253 13.396 1.00 26.19 ATOM 1902 O VAL 1093 41.618 15.235 12.938 1.00 23.95 ATOM 1903 N LEU 1094 40.363 15.893 12.484 1.00 19.63 ATOM 1905 CA LEU 1094 40.667 17.338 12.050 1.00 25.24 ATOM 1906 CB LEU 1094 39.587 18.420 11.974 1.00 27.30 ATOM 1907 CG LEU 1094 40.136 19.497 11.113 1.00 28.26 ATOM 1908 CD1 LEU 1094 38.265 17.929 11.385 1.00 27.54 ATOM 1909 CD2 LEU 1094 39.775 15.146 11.280 1.00 16.12 ATOM 1910 C LEU 1094 38.555 15.002 11.129 1.00 16.14 ATOM 1911 O LEU 1094 40.631 14.766 10.348 1.00 16.30 ATOM 1912 N LEU 1095 40.155 14.003 9.195 1.00 17.98 ATOM 1914 CA LEU 1095 41.321 13.538 8.317 1.00 16.52 ATOM 1915 CB LEU 1095 41.981 14.536 7.386 1.00 14.88 ATOM 1916 CG LEU 1095 42.807 13.734 6.399 1.00 11.81 ATOM 1917 CD1 LEU 1095 40.931 15.401 6.639 1.00 21.08 ATOM 1918 CD2 LEU 1095 39.437 12.770 9.722 1.00 17.52 ATOM 1919 C LEU 1095 38.324 12.448 9.270 1.00 16.23 ATOM 1920 O LEU 1095 40.077 12.105 10.697 1.00 14.50 ATOM 1921 N TRP 1096 39.509 10.916 11.304 1.00 14.02 ATOM 1923 CA TRP 1096 40.452 10.330 12.337 1.00 13.21 ATOM 1924 CB TRP 1096 ATOM 1925 CG TRP 1096 40.010 8.992 12.850 1.00 18.93 39.016 8.732 13.856 1.00 24.77 ATOM 1926 CD2 TRP 1096 ATOM 1927 CE2 TRP 1096 38.952 7.319 14.020 1.00 27.07 38.178 9.546 14.647 1.00 29.39 ATOM 1928 CE3 TRP 1096 40.483 7.781 12.460 1.00 21.28 ATOM 1929 CD1 TRP 1096 - 39.854 6.770 13.154 1.00 18.61 ATOM 1930 NE1 TRP 1096 38.075 6.700 14.954 1.00 28.21 ATOM 1932 CZ2 TRP 1096 37.303 8.927 15.581 1.00 29.42 ATOM 1933 CZ3 TRP 1096 37.266 7.511 15.719 1.00 27.60 ATOM 1934 CH2 TRP 1096

FIG. 7(39)

38.159 11.236 11.927 1.00 18.94 ATOM 1935 C TRP 1096 37.212 10.439 11.826 1.00 22.31 ATOM 1936 O TRP 1096 38.046 12.385 12.592 1.00 23.97 ATOM 1937 N GLU 1097 36.754 12.750 13.195 1.00 21.61 ATOM 1939 CA GLU 1097 36.823 14.012 14.041 1.00 26.60 ATOM 1940 CB GLU 1097 37.880 14.065 15.109 1.00 21.55 ATOM 1941 CG GLU 1097 37.795 15.380 15.800 1.00 23.56 ATOM 1942 CD GLU 1097 ATOM 1943 OE1 GLU 1097 36.726 15.591 16.393 1.00 21.97 38.741 16.208 15.706 1.00 20.79 ATOM 1944 OE2 GLU 1097 35.744 13.010 12.116 1.00 19.15 ATOM 1945 C GLU 1097 34.549 12.766 12.304 1.00 28.35 ATOM 1946 O GLU 1097 36.190 13.565 11.001 1.00 17.99 ATOM 1947 N ILE 1098 ATOM 1949 CA ILE 1098 35.244 13.821 9.915 1.00 17.98 35.862 14.650 8.732 1.00 13.59 ATOM 1950 CB ILE 1098 34.880 14.725 7.568 1.00 13.47 ATOM 1951 CG2 ILE 1098 36.169 16.074 9.181 1.00 11.46 ATOM 1952 CG1 ILE 1098 36.691 16.960 8.074 1.00 9.72 ATOM 1953 CD1 ILE 1098 34.645 12.529 9.372 1.00 16.07 ATOM 1954 C ILE 1098 33.444 12.445 9.171 1.00 18.22 ATOM 1955 O ILE 1098 35.460 11.499 9.171 1.00 20.11 ATOM 1956 N PHE 1099 34.925 10.257 8.601 1.00 18.95 ATOM 1958 CA PHE 1099 35.909 9.660 7.625 1.00 16.86 ATOM 1959 CB PHE 1099 36.269 10.584 6.517 1.00 12.61 ATOM 1960 CG PHE 1099 37.308 11.468 6.671 1.00 14.37 ATOM 1961 CD1 PHE 1099 35.522 10.624 5.362 1.00 18.03 ATOM 1962 CD2 PHE 1099 37.595 12.369 5.717 1.00 13.66 ATOM 1963 CE1 PHE 1099 35.811 11.553 4.378 1.00 16.05 ATOM 1964 CE2 PHE 1099 36.843 12.418 4.568 1.00 17.86 ATOM 1965 CZ PHE 1099 34.368 9.201 9.551 1.00 23.18 ATOM 1966 C PHE 1099 34.111 8.070 9.149 1.00 22.90 ATOM 1967 O PHE 1099 34.274 9.553 10.825 1.00 26.68 ATOM 1968 N SER 1100 33.652 8.690 11.820 1.00 24.51 ATOM 1970 CA SER 1100 34.504 8.572 13.079 1.00 25.60 ATOM 1971 CB SER 1100 34.826 9.842 13.625 1.00 29.76 ATOM 1972 OG SER 1100 32.398 9.465 12.145 1.00 26.92 ATOM 1974 C SER 1100 31.765 9.211 13.157 1.00 31.32 ATOM 1975 O SER 1100 32.018 10.387 11.251 1.00 28.15 1976 N LEU 1101 MOTA 30.860 11.241 11.453 1.00 24.97 ATOM 1978 CA LEU 1101 30.860 11.241 11.453 1.00 24.97 29.556 10.557 11.015 1.00 22.00 1979 CB LEU 1101 MOTA 29.423 10.410 9.495 1.00 25.66 ATOM 1980 CG LEU 1101

FIG. 7(40)

28.060 9.866 9.127 1.00 22.23 ATOM 1981 CD1 LEU 1101 29.632 11.768 8.829 1.00 32.30 ATOM 1982 CD2 LEU 1101 30.771 11.779 12.888 1.00 26.64 ATOM 1983 C LEU 1101 29.793 11.552 13.580 1.00 31.34 ATOM 1984 O LEU 1101 31.828 12.446 13.336 1.00 24.93 ATOM 1985 N GLY 1102 31.836 13.057 14.650 1.00 28.61 ATOM 1987 CA GLY 1102 32.129 12.293 15.917 1.00 32.38 ATOM 1988 C GLY 1102 31.647 12.693 16.950 1.00 35.69 ATOM 1989 O GLY 1102 33.004 11.291 15.876 1.00 35.95 ATOM 1990 N ALA 1103 33.354 10.500 17.060 1.00 31.27 ATOM 1992 CA ALA 1103 33.515 9.041 16.672 1.00 36.15 ATOM 1993 CB ALA 1103 34.625 10.972 17.747 1.00 34.29 ATOM 1994 C ALA 1103 35.382 11.788 17.190 1.00 36.92 ATOM 1995 O ALA 1103 34.886 10.417 18.934 1.00 33.11 ATOM 1996 N SER 1104 36.087 10.744 19.715 1.00 35.13 ATOM 1998 CA SER 1104 35.906 10.422 21.207 1.00 38.40 ATOM 1999 CB SER 1104 34.719 10.964 21.765 1.00 50.36 ATOM 2000 OG SER 1104 37.216 9.852 19.249 1.00 34.54 ATOM- 2002 C SER 1104 37.039 8.640 19.167 1.00 33.44 ATOM 2003 O SER 1104 38.395 10.434 18.963 1.00 32.93 ATOM 2004 N PRO 1105 38.678 11.877 18.972 1.00 31.54 ATOM 2005 CD PRO 1105 ATOM 2006 CA PRO 1105 39.571 9.693 18.513 1.00 29.88 40.633 10.781 18.465 1.00 22.24 ATOM 2007 CB PRO 1105 39.883 11.965 18.079 1.00 28.04 ATOM 2008 CG PRO 1105 39.919 8.659 19.582 1.00 32.54 ATOM 2009 C PRO 1105 39.480 8.795 20.731 1.00 28.79 ATOM 2010 O PRO 1105 40.700 7.648 19.196 1.00 34.52 ATOM 2011 N TYR 1106 41.148 6.564 20.085 1.00 39.62 ATOM 2013 CA TYR 1106 42.374 6.994 20.896 1.00 37.66 ATOM 2014 CB TYR 1106 43.496 7.566 20.059 1.00 39.50 ATOM 2015 CG TYR 1106 43.690 8.957 19.976 1.00 37.50 ATOM 2016 CD1 TYR 1106 44.655 9.518 19.143 1.00 35.61 ATOM 2017 CE1 TYR 1106 44.315 6.739 19.293 1.00 34.54 ATOM 2018 CD2 TYR 1106 45.305 7.290 18.446 1.00 38.80 ATOM 2019 CE2 TYR 1106 45.466 8.686 18.373 1.00 38.23 ATOM 2020 CZ TYR 1106 46.412 9.240 17.520 1.00 31.37 ATOM 2021 OH TYR 1106 40.022 6.128 21.016 1.00 47.24-ATOM 2023 C TYR 1106 40.100 6.296 22.247 1.00 46.94 ATOM 2024 O TYR 1106 38.947 5.570 20.431 1.00 52.30 ATOM 2025 N PRO 1107 38.880 5.234 18.996 1.00 52.76 ATOM 2026 CD PRO 1107

FIG. 7(41)

37.750 5.088 21.125 1.00 55.67 ATOM 2027 CA PRO 1107 37.078 4.223 20.066 1.00 55.09 ATOM 2028 CB PRO 1107 37.420 4.931 18.797 1.00 52.62 ATOM 2029 CG PRO 1107 38.035 4.300 22.408 1.00 60.55 ATOM 2030 C PRO 1107 38.668 3.231 22.377 1.00 60.88 ATOM 2031 O PRO 1107 37.631 4.894 23.533 1.00 62.85 ATOM 2032 N GLY 1108 ATOM 2034 CA GLY 1108 37.790 4.284 24.845 1.00 63.10 39.171 3.783 25.228 1.00 61.44 ATOM 2035 C GLY 1108 39.319 3.010 26.178 1.00 63.49 ATOM 2036 O GLY 1108

 39.319
 3.010
 26.178
 1.00 63.49

 40.181
 4.228
 24.498
 1.00 58.31

 41.548
 3.835
 24.766
 1.00 55.54

 42.430
 4.181
 23.580
 1.00 54.11

 43.857
 3.787
 23.857
 1.00 51.33

 41.875
 3.528
 22.306
 1.00 54.09

 ATOM 2037 N VAL 1109 ATOM 2039 CA VAL 1109 ATOM 2040 CB VAL 1109 ATOM 2041 CG1 VAL 1109 ATOM 2042 CG2 VAL 1109 42.006 4.657 25.949 1.00 57.04 ATOM 2043 C VAL 1109 42.006 4.657 25.949 1.00 57.04 41.492 5.749 26.163 1.00 57.18 42.969 4.140 26.711 1.00 59.43 ATOM 2044 O VAL 1109 ATOM 2045 N LYS 1110

 43.497
 4.849
 27.880
 1.00 60.27

 43.928
 3.842
 28.936
 1.00 63.70

 44.664
 5.796
 27.538
 1.00 60.52

 45.570
 5.410
 26.780
 1.00 61.06

 44.665
 7.006
 28.115
 1.00 58.79

 45.732
 7.987
 27.859
 1.00 60.01

 45.236
 9.441
 27.886
 1.00 63.41

 44.517
 9.798
 26.596
 1.00 58.31

 44.413
 9.688
 29.145
 1.00 69.87

 43.497 4.849 27.880 1.00 60.27 ATOM 2047 CA LYS 1110 ATOM 2048 CB LYS 1110 ATOM 2049 C LYS 1110 ATOM 2050 O LYS 1110 ATOM 2051 N ILE 1111 ATOM 2053 CA ILE 1111 ATOM 2054 CB ILE 1111 ATOM 2055 CG2 ILE 1111 ATOM 2056 CG1 ILE 1111 44.341 11.144 29.528 1.00 75.64 ATOM 2057 CD1 ILE 1111 46.949 7.891 28.781 1.00 58.91 ATOM 2058 C ILE 1111 ATOM 2059 O ILE 1111 ATOM 2060 N ASP 1112 ATOM 2062 CA ASP 1112 ATOM 2063 CB ASP 1112 ATOM 2064 CG ASP 1112 ATOM 2065 OD1 ASP 1112 49.348 3.765 28.628 1.00 72.11 ATOM 2066 OD2 ASP 1112 49.612 6.795 29.489 1.00 54.37 ATOM 2067 C ASP 1112 49.634 7.066 28.284 1.00 50.67 50.710 6.741 30.236 1.00 55.36 52.024 7.089 29.683 1.00 55.99 53.051 7.374 30.806 1.00 58.69 ATOM 2068 O ASP 1112 ATOM 2069 N GLU 1113 ATOM 2071 CA GLU 1113 ATOM 2072 CB GLU 1113

FIG. 7(42)

52.552 6.015 28.726 1.00 54.42 ATOM 2073 C GLU 1113 ATOM 2074 O GLU 1113 53.624 6.175 28.126 1.00 51.91 51.822 4.903 28.627 1.00 51.54 ATOM 2075 N GLU 1114 52.192 3.819 27.719 1.00 54.36 ATOM 2077 CA GLU 1114 51.873 2.452 28.322 1.00 56.43 ATOM 2078 CB GLU 1114 ATOM 2079 CG GLU 1114 53.072 1.749 28.948 1.00 63.29 53.996 2.661 29.772 1.00 67.36 ATOM 2080 CD GLU 1114 55.153 2.870 29.329 1.00 67.34 ATOM 2081 OE1 GLU 1114 53.590 3.127 30.873 1.00 68.20 ATOM 2082 OE2 GLU 1114 51.440 4.031 26.412 1.00 52.22 ATOM 2083 C GLU 1114 51.830 3.514 25.360 1.00 51.74 ATOM 2084 O GLU 1114 ATOM 2085 N PHE 1115 50.383 4.840 26.486 1.00 49.67 49.603 5.175 25.320 1.00 44.59 ATOM 2087 CA PHE 1115 48.400 6.013 25.688 1.00 44.73 47.918 6.890 24.579 1.00 49.93 ATOM 2088 CB PHE 1115 ATOM 2089 CG PHE 1115 48.140 8.270 24.621 1.00 50.02 ATOM 2090 CD1 PHE 1115 47.251 6.344 23.477 1.00 53.38 ATOM 2091 CD2 PHE 1115 47.704 9.098 23.577 1.00 52.88 ATOM 2092 CE1 PHE 1115 ATOM 2093 CE2 PHE 1115 46.805 7.158 22.425 1.00 51.00 ATOM 2094 CZ PHE 1115 47.033 8.535 22.474 1.00 54.64 50.582 5.981 24.507 1.00 46.08 ATOM 2095 C PHE 1115 ATOM 2096 O PHE 1115 50.929 5.572 23.402 1.00 47.48 51.127 7.047 25.101 1.00 43.91 ATOM 2097 N CYS 1116 52.109 7.898 24.404 1.00 45.79 ATOM 2099 CA CYS 1116 52.473 9.113 25.247 1.00 44.47 ATOM 2100 CB CYS 1116 51.129 9.723 26.295 1.00 64.10 ATOM 2101 SG CYS 1116 53.392 7.140 24.019 1.00 46.03 ATOM 2102 C CYS 1116 54.232 7.667 23.279 1.00 46.86 53.536 5.911 24.529 1.00 44.91 54.232 7.667 23.279 1.00 46.86 ATOM 2103 O CYS 1116 ATOM 2104 N ARG 1117

 53.536
 5.911
 24.529
 1.00 44.91

 54.688
 5.069
 24.237
 1.00 41.89

 54.882
 4.001
 25.308
 1.00 43.78

 56.237
 3.298
 25.233
 1.00 45.19

 56.189
 1.905
 25.856
 1.00 47.09

 55.490
 0.922
 25.021
 1.00 49.55

 54.329
 0.337
 25.336
 1.00 51.59

 53.783
 -0.547
 24.506
 1.00 51.49

 53.695
 0.649
 26.461
 1.00 47.17

 54.370
 4.389
 22.927
 1.00 38.98

 55.156
 4.455
 21.996
 1.00 42.49

 53.206
 3.751
 22.860
 1.00 35.52

 ATOM 2106 CA ARG 1117 ATOM 2107 CB ARG 1117 ATOM 2108 CG ARG 1117 ATOM 2109 CD ARG 1117 ATOM 2110 NE ARG 1117 ATOM 2112 CZ ARG 1117 ATOM 2113 NH1 ARG 1117 ATOM 2116 NH2 ARG 1117 ATOM 2119 C ARG 1117 ATOM 2120 O ARG 1117 53.206 3.751 22.860 1.00 35.52 ATOM 2121 N ARG 1118

FIG. 7(43)

52.745 3.072 21.649 1.00 36.78 ATOM 2123 CA ARG 1118 ATOM 2124 CB ARG 1118 51.330 2.559 21.880 1.00 31.14 ATOM 2125 CG ARG 1118 51.216 1.675 23.068 1.00 34.41 49.766 1.587 23.535 1.00 45.83 ATOM 2126 CD ARG 1118 48.897 0.750 22.693 1.00 53.41 ATOM 2127 NE ARG 1118 ATOM 2129 CZ ARG 1118 47.564 0.658 22.826 1.00 55.58 46.862 -0.144 22.025 1.00 56.70 ATOM 2130 NH1 ARG 1118 ATOM 2133 NH2 ARG 1118 46.921 1.380 23.745 1.00 55.55 52.742 4.067 20.471 1.00 38.92 ATOM 2136 C ARG 1118 53.331 3.835 19.400 1.00 38.28 ATOM 2137 O ARG 1118 52.063 5.186 20.711 1.00 40.67 ATOM 2138 N LEU 1119 ATOM 2140 CA LEU 1119 51.912 6.295 19.779 1.00 36.71 ATOM 2141 CB LEU 1119 51.192 7.416 20.540 1.00 32.46 50.238 8.508 20.049 1.00 25.91 ATOM 2142 CG LEU 1119 51.047 9.651 19.564 1.00 19.62 ATOM 2143 CD1 LEU 1119 ATOM 2144 CD2 LEU 1119 49.250 7.993 19.024 1.00 22.26 ATOM 2145 C LEU 1119 53.301 6.728 19.245 1.00 38.89 53.469 6.960 18.047 1.00 43.59 ATOM 2146 O LEU 1119 54.315 6.771 20.099 1.00 42.22 ATOM 2147 N LYS 1120 ATOM 2149 CA LYS 1120 55.649 7.152 19.640 1.00 41.56 56.523 7.548 20.813 1.00 42.85 ATOM 2150 CB LYS 1120 57.467 8.670 20.467 1.00 52.51 ATOM 2151 CG LYS 1120 58.407 8.989 21.620 1.00 60.23 ATOM 2152 CD LYS 1120 59.298 10.206 21.321 1.00 69.72 ATOM 2153 CE LYS 1120 ATOM 2154 NZ LYS 1120 58.605 11.557 21.283 1.00 76.23 ATOM 2158 C LYS 1120 56.351 6.050 18.825 1.00 43.73 57.287 6.342 18.073 1.00 47.49 ATOM 2159 O LYS 1120 55.892 4.800 18.966 1.00 43.94 ATOM 2160 N GLU 1121 ATOM 2162 CA GLU 1121 56.453 3.636 18.262 1.00 41.07 56.415 2.395 19.147 1.00 48.40 ATOM 2163 CB GLU 1121 ATOM 2164 CG GLU 1121 57.553 2.283 20.112 1.00 58.39 57.183 1.451 21.309 1.00 64.79 ATOM 2165 CD GLU 1121 56.403 0.483 21.119 1.00 67.43 ATOM 2166 OE1 GLU 1121 ATOM 2167 OE2 GLU 1121 57.657 1.778 22.431 1.00 67.24 55.739 3.284 16.968 1.00 39.16 56.224 2.423 16.216 1.00 39.90 54.525 3.805 16.781 1.00 31.72 ATOM 2168 C GLU 1121 ATOM 2169 O GLU 1121 ATOM 2170 N GLY 1122 53.838 3.550 15.531 1.00 22.36 ATOM 2172 CA GLY 1122 -52.427 3.064 15.646 1.00 19.85 ATOM 2173 C GLY 1122 51.791 2.779 14.633 1.00 18.01 ATOM 2174 O GLY 1122

FIG. 7(44)

ATOM 2175 N THR 1123 51.918 2.946 16.860 1.00 16.84 50.535 2.502 16.989 1.00 22.17 ATOM 2177 CA THR 1123 ATOM 2178 CB THR 1123 50.209 2.144 18.469 1.00 29.75 51.148 1.174 18.971 1.00 31.60 ATOM 2179 OG1 THR 1123 48.794 1.587 18.591 1.00 31.44 ATOM 2181 CG2 THR 1123 ATOM 2182 C THR 1123 49.653 3.673 16.453 1.00 23.74 49.940 4.850 16.721 1.00 18.73 ATOM 2183 O THR 1123 48.597 3.354 15.701 1.00 22.93 ATOM 2184 N ARG 1124 47.735 4.379 15.125 1.00 17.39 48.094 4.680 13.670 1.00 17.70 49.478 5.192 13.406 1.00 14.57 49.713 6.484 14.040 1.00 14.31 ATOM 2186 CA ARG 1124 ATOM 2187 CB ARG 1124 ATOM 2188 CG ARG 1124 ATOM 2189 CD ARG 1124 49.713 6.484 14.040 1.00 14.31 49.713 6.484 14.040 1.00 14.31 51.046 6.935 13.684 1.00 10.98 52.067 6.988 14.533 1.00 16.02 51.861 6.604 15.775 1.00 10.96 53.269 7.468 14.163 1.00 8.74 46.317 3.893 15.096 1.00 16.31 ATOM 2190 NE ARG 1124 ATOM 2192 CZ ARG 1124 ATOM 2193 NH1 ARG 1124 ATOM 2196 NH2 ARG 1124 ATOM 2199 C ARG 1124 46.085 2.698 15.022 1.00 20.38 45.380 4.847 15.081 1.00 21.15 43.943 4.570 15.023 1.00 23.81 43.158 5.870 15.012 1.00 16.88 42.783 6.397 16.380 1.00 17.08 41.656 7.825 16.270 1.00 25.19 42.908 9.123 15.776 1.00 17.02 ATOM 2200 O ARG 1124 ATOM 2201 N MET 1125 ATOM 2203 CA MET 1125 ATOM 2204 CB MET 1125 ATOM 2205 CG MET 1125 ATOM 2206 SD MET 1125 ATOM 2207 CE MET 1125 ATOM 2208 C MET 1125 43.604 3.789 13.749 1.00 29.80

 44.298
 3.923
 12.748
 1.00
 33.37

 42.576
 2.953
 13.806
 1.00
 36.07

 42.116
 2.183
 12.668
 1.00
 36.36

 41.465
 0.859
 13.154
 1.00
 40.10

 40.257
 1.021
 14.061
 1.00
 54.46

 38.956
 1.268
 13.263
 1.00
 65.08

 37.839
 1.758
 14.091
 1.00
 72.39

 36.545
 1.753
 13.740
 1.00
 74.53

 35.636
 2.233
 14.588
 1.00
 78.72

 36.140
 1.267
 12.562
 1.00
 74.28

 ATOM 2209 O MET 1125 ATOM 2210 N ARG 1126 ATOM 2212 CA ARG 1126 ATOM 2213 CB ARG 1126 ATOM 2214 CG ARG 1126 ATOM 2215 CD ARG 1126 ATOM 2216 NE ARG 1126 ATOM 2218 CZ ARG 1126 ATOM 2219 NH1 ARG 1126 36.140 1.267 12.562 1.00 74.28 41.124 3.094 11.888 1.00 32.52 40.706 4.117 12.380 1.00 34.88 40.760 2.725 10.676 1.00 29.80 39.888 3.508 9.812 1.00 29.83 39.743 2.782 8.460 1.00 32.24 ATOM 2222 NH2 ARG 1126 ATOM 2225 C ARG 1126 ATOM 2226 O ARG 1126 ATOM 2227 N ALA 1127 ATOM 2229 CA ALA 1127 ATOM 2230 CB ALA 1127

FIG. 7(45)

ATOM 2231 C ALA 1127 38.518 3.697 10.415 1.00 34.29 37.944 2.727 10.881 1.00 39.95 ATOM 2232 O ALA 1127 37.943 4.934 10.335 1.00 34.66 ATOM 2233 N PRO 1128 ATOM 2234 CD PRO 1128 38.477 6.142 9.685 1.00 35.04 36.612 5.251 10.871 1.00 31.59 ATOM 2235 CA PRO 1128 36.511 6.776 10.669 1.00 32.56 ATOM 2236 CB PRO 1128 ATOM 2237 CG PRO 1128 37.819 7.222 10.499 1.00 31.06 35.648 4.597 9.916 1.00 33.99 ATOM 2238 C PRO 1128 35.975 4.429 8.749 1.00 38.28 ATOM 2239 O PRO 1128 34.416 4.371 10.344 1.00 31.98 ATOM 2240 N ASP 1129 33.425 3.728 9.489 1.00 34.11 ATOM 2242 CA ASP 1129 32.157 3.432 10.277 1.00 29.91 ATOM 2243 CB ASP 1129 ATOM 2244 CG ASP 1129 32.447 2.811 11.623 1.00 34.04 33.519 2.172 11.805 1.00 35.22 ATOM 2245 OD1 ASP 1129 31.597 2.976 12.515 1.00 36.43 ATOM 2246 OD2 ASP 1129 ATOM 2247 C ASP 1129 33.061 4.360 8.158 1.00 35.75 32.441 3.699 7.312 1.00 38.26 ATOM 2248 O ASP 1129 33.444 5.613 7.925 1.00 32.58 ATOM 2249 N TYR 1130 ATOM 2251 CA TYR 1130 33.056 6.200 6.649 1.00 34.86 32.067 7.332 6.888 1.00 38.26 ATOM 2252 CB TYR 1130 ATOM 2253 CG TYR 1130 30.996 6.960 7.889 1.00 37.51 31.208 7.153 9.245 1.00 36.44 ATOM 2254 CD1 TYR 1130 ATOM 2255 CE1 TYR 1130 30.249 6.853 10.148 1.00 40.00 ATOM 2256 CD2 TYR 1130 29.787 6.442 7.468 1.00 39.18 28.813 6.143 8.360 1.00 34.53 ATOM 2257 CE2 TYR 1130 29.050 6.353 9.709 1.00 39.16 ATOM 2258 CZ TYR 1130 28.120 6.147 10.690 1.00 47.34 ATOM 2259 OH TYR 1130 34.136 6.657 5.732 1.00 34.80 ATOM 2261 C TYR 1130 33.853 7.257 4.694 1.00 27.05 ATOM 2262 O TYR 1130 ATOM 2263 N THR 1131 35.388 6.414 6.108 1.00 37.58 36.457 6.829 5.238 1.00 38.70 ATOM 2265 CA THR 1131 ATOM 2266 CB THR 1131 37.783 6.598 5.763 1.00 39.57 37.775 5.417 6.564 1.00 51.23 ATOM 2267 OG1 THR 1131 ATOM 2269 CG2 THR 1131 38.250 7.775 6.481 1.00 49.58 ATOM 2270 C THR 1131 36.476 6.071 3.955 1.00 38.19 35.913 4.967 3.808 1.00 38.82 ATOM 2271 O THR 1131 37.297 6.649 3.104 1.00 31.58 ATOM 2272 N THR 1132 37.638 6.148 1.836 1.00 27.37 ATOM 2274 CA THR 1132 37.591 7.302 0.887 1.00 18.06 ATOM 2275 CB THR 1132 ATOM 2276 OG1 THR 1132 36.274 7.366 0.348 1.00 29.75

FIG. 7(46)

ATOM 2278 CG2 THR 1132 38.528 7.126 -0.161 1.00 32.09 39.064 5.634 2.159 1.00 31.18 ATOM 2279 C THR 1132 ATOM 2280 O THR 1132 39.678 6.088 3.149 1.00 37.35 39.543 4.601 1.439 1.00 29.49 ATOM 2281 N PRO 1133 38.884 3.875 0.336 1.00 28.18 ATOM 2282 CD PRO 1133 ATOM 2283 CA PRO 1133 40.876 4.065 1.686 1.00 23.60 ATOM 2284 CB PRO 1133 41.029 2.998 0.604 1.00 29.05 39.640 2.581 0.319 1.00 28.36 ATOM 2285 CG PRO 1133 41.917 5.122 1.500 1.00 22.87 ATOM 2286 C PRO 1133 42.944 5.119 2.182 1.00 30.07 41.700 5.983 0.511 1.00 18.80 ATOM 2287 O PRO 1133 ATOM 2288 N GLU 1134 42.656 7.049 0.264 1.00 22.21 42.594 7.573 -1.160 1.00 26.28 41.214 7.564 -1.765 1.00 40.23 40.901 6.347 -2.617 1.00 42.05 41.727 6.004 -3.504 1.00 44.65 39.799 5.779 -2.453 1.00 44.07 ATOM 2290 CA GLU 1134 ATOM 2291 CB GLU 1134 ATOM 2292 CG GLU 1134 ATOM 2293 CD GLU 1134 ATOM 2294 OE1 GLU 1134 ATOM 2295 OE2 GLU 1134 42.547 8.164 1.300 1.00 21.07 ATOM 2296 C GLU 1134 ATOM 2297 O GLU 1134 43.528 8.877 1.543 1.00 20.78 41.375 8.304 1.940 1.00 20.24 41.233 9.304 2.996 1.00 16.52 39.775 9.658 3.319 1.00 17.57 39.158 10.807 2.420 1.00 15.02 40.199 12.320 2.187 1.00 20.17 ATOM 2298 N MET 1135 ATOM 2300 CA MET 1135 ATOM 2301 CB MET 1135 ATOM 2302 CG MET 1135 39.158 10.807 2.420 1.00 15.02 40.199 12.320 2.187 1.00 20.17 ATOM 2303 SD MET 1135 ATOM 2304 CE MET 1135 40.632 12.648 3.877 1.00 13.20 41.974 8.751 4.191 1.00 20.41 ATOM 2305 C MET 1135 42.772 9.461 4.787 1.00 25.79 ATOM 2306 O MET 1135 41.836 7.448 4.445 1.00 20.30 ATOM 2307 N TYR 1136 ATOM 2309 CA TYR 1136

 42.565
 6.817
 5.540
 1.00
 17.65

 42.082
 5.394
 5.832
 1.00
 21.89

 42.786
 4.775
 7.041
 1.00
 26.17

 42.565 6.817 5.540 1.00 17.65 ATOM 2310 CB TYR 1136 ATOM 2311 CG TYR 1136 42.702 5.353 8.325 1.00 20.81 ATOM 2312 CD1 TYR 1136 43.364 4.781 9.427 1.00 17.33 ATOM 2313 CE1 TYR 1136 43.554 3.612 6.900 1.00 26.03 44.225 3.034 7.998 1.00 12.75 ATOM 2314 CD2 TYR 1136 ATOM 2315 CE2 TYR 1136 44.124 3.615 9.245 1.00 16.64 44.791 2.999 10.281 1.00 17.57 44.077 6.847 5.267 1.00 14.28 44.892 7.066 6.179 1.00 19.62 ATOM 2316 CZ TYR 1136 44.791 2.999 10.281 1.00 17.57 ATOM 2317 OH TYR 1136 ATOM 2319 C TYR 1136 ATOM 2320 O TYR 1136 44.479 6.693 4.022 1.00 12.55 ATOM 2321 N GLN 1137

FIG. 7(47)

ATOM 2323 CA GLN 1137 45.903 6.777 3.758 1.00 16.34 46.2186.4122.3251.0018.3647.7026.6541.9451.0021.7948.6135.6552.5611.0014.21 ATOM 2324 CB GLN 1137 ATOM 2325 CG GLN 1137 ATOM 2326 CD GLN 1137 ATOM 2327 OE1 GLN 1137 48.416 4.469 2.381 1.00 22.64 ATOM 2328 NE2 GLN 1137 49.571 6.111 3.344 1.00 18.97 46.415 8.193 4.041 1.00 20.40 ATOM 2331 C GLN 1137 47.598 8.378 4.391 1.00 25.11 ATOM 2332 O GLN 1137 ATOM 2333 N THR 1138 45.564 9.194 3.807 1.00 18.65 ATOM 2335 CA THR 1138 45.939 10.568 4.068 1.00 15.52 ATOM 2336 CB THR 1138 44.921 11.507 3.538 1.00 19.97 44.797 11.257 2.144 1.00 18.74 ATOM 2337 OG1 THR 1138 45.381 12.939 3.722 1.00 21.70 ATOM 2339 CG2 THR 1138 ATOM 2340 C THR 1138 46.111 10.721 5.566 1.00 12.73 ATOM 2341 O THR 1138 47.067 11.344 6.010 1.00 18.83 45.233 10.118 6.352 1.00 9.32 ATOM 2342 N MET 1139 45.402 10.151 7.809 1.00 12.25 44.295 9.349 8.480 1.00 13.21 ATOM 2344 CA MET 1139 44.295 9.349 8.480 1.00 13.21 42.967 10.007 8.354 1.00 5.60 41.708 8.982 9.003 1.00 17.66 40.510 9.337 7.925 1.00 2.00 46.773 9.567 8.198 1.00 15.96 47.573 10.237 8.855 1.00 17.30 47.058 8.333 7.770 1.00 15.29 48.357 7.735 8.081 1.00 15.29 ATOM 2345 CB MET 1139 ATOM 2346 CG MET 1139 ATOM 2347 SD MET 1139 ATOM 2348 CE MET 1139 ATOM 2349 C MET 1139 ATOM 2350 O MET 1139 ATOM 2351 N LEU 1140 ATOM 2353 CA LEU 1140 48.542 6.409 7.326 1.00 6.27 47.511 5.373 7.745 1.00 15.42 ATOM 2354 CB LEU 1140 ATOM 2355 CG LEU 1140 47.511 5.373 7.745 1.00 15.42 47.656 4.103 6.927 1.00 8.64 ATOM 2356 CD1 LEU 1140 ATOM 2357 CD2 LEU 1140 47.648 5.103 9.246 1.00 14.99 49.518 8.684 7.751 1.00 17.20 ATOM 2358 C LEU 1140 ATOM 2359 O LEU 1140 50.552 8.691 8.442 1.00 18.73 ATOM 2360 N ASP 1141 49.396 9.413 6.644 1.00 20.16 50.442 10.374 6.229 1.00 19.52 50.139 10.963 4.851 1.00 20.89 ATOM 2362 CA ASP 1141 ATOM 2363 CB ASP 1141 ATOM 2364 CG ASP 1141 50.228 9.942 3.772 1.00 25.01 50.537 8.765 4.074 1.00 30.17 49.994 10.321 2.624 1.00 26.42 50.537 8.765 4.074 1.00 30.17 ATOM 2365 OD1 ASP 1141 ATOM 2366 OD2 ASP 1141 50.627 11.521 7.207 1.00 15.10 ATOM 2367 C ASP 1141 51.762 11.905 7.502 1.00 8.73 ATOM 2368 O ASP 1141 ATOM 2369 N CYS 1142 49.504 12.101 7.637 1.00 10.75

FIG. 7(48)

ATOM 2371 CA CYS 1142 ATOM 2372 CB CYS 1142 ATOM 2373 SG CYS 1142 ATOM 2374 C CYS 1142 ATOM 2375 O CYS 1142 ATOM 2376 N TRP 1143 ATOM 2378 CA TRP 1143 ATOM 2379 CB TRP 1143 ATOM 2380 CG TRP 1143 ATOM 2381 CD2 TRP 1143 ATOM 2382 CE2 TRP 1143 ATOM 2383 CE3 TRP 1143 ATOM 2384 CD1 TRP 1143 ATOM 2385 NE1 TRP 1143 ATOM 2387 CZ2 TRP 1143 ATOM 2388 CZ3 TRP 1143 ATOM 2389 CH2 TRP 1143 ATOM 2390 C TRP 1143 ATOM 2391 O TRP 1143 ATOM 2392 N HIS 1144 ATOM 2394 CA HIS 1144 ATOM 2395 CB HIS 1144 ATOM 2396 CG HIS 1144 ATOM 2397 CD2 HIS 1144 ATOM 2398 ND1 HIS 1144 ATOM 2400 CE1 HIS 1144 ATOM 2401 NE2 HIS 1144 ATOM 2403 C HIS 1144 ATOM 2404 O HIS 1144 ATOM 2405 N GLY 1145 ATOM 2407 CA GLY 1145 ATOM 2408 C GLY 1145 ATOM 2409 O GLY 1145 ATOM 2410 N GLU 1146 ATOM 2412 CA GLU 1146 ATOM 2413 CB GLU 1146 ATOM 2414 CG GLU 1146 ATOM 2415 CD GLU 1146 ATOM 2416 OE1 GLU 1146 ATOM 2417 OE2 GLU 1146

49.516 13.196 8.590 1.00 13.88 48.110 13.776 8.739 1.00 17.83 48.110 13.776 8.739 1.00 17.83 47.414 14.574 7.291 1.00 17.66 50.042 12.717 9.961 1.00 15.52 50.545 13.513 10.734 1.00 16.31 49.883 11.424 10.266 1.00 20.06 50.344 10.830 11.528 1.00 17.66 49.393 9.727 11.991 1.00 15.44 48.041 10.236 12.273 1.00 14.25 46.814 9.495 12.233 1.00 18.13 45.774 10.401 12.540 1.00 12.59 46.490 8.143 11.966 1.00 16.02 47.710 11.514 12.605 1.00 7.90 46.355 11.618 12.768 1.00 13.52 44.425 10.012 12.592 1.00 8.83 45.155 7.755 12.017 1.00 11.61 44.133 8.691 12.327 1.00 16.83 45.155 7.755 12.017 1.00 11.61
44.133 8.691 12.327 1.00 16.83
51.765 10.281 11.442 1.00 23.22
52.208 9.507 12.298 1.00 27.31
52.510 10.722 10.440 1.00 24.48
53.876 10.280 10.299 1.00 26.08
54.495 10.859 9.023 1.00 19.25
55.791 10.214 8.654 1.00 18.57
56.923 10.003 9.374 1.00 14.60
56.016 9.657 7.415 1.00 19.61
57.231 9.133 7.387 1.00 19.99
57.803 9.332 8.562 1.00 15.04
54.710 10.671 11.542 1.00 32.65
54.626 11.795 12.031 1.00 31.70
55.541 9.734 12.016 1.00 37.26
56.393 9.970 13.168 1.00 31.32
57.251 11.212 13.001 1.00 35.04
57.372 11.989 13.942 1.00 38.42
57.915 11.373 11.852 1.00 34.51
58.735 12.577 11.598 1.00 37.16
59.871 12.303 10.627 1.00 37.16
61.093 11.742 11.292 1.00 50.26
61.186 10.243 11.110 1.00 54.17
61.158 9.509 12.125 1.00 55.25
61.280 9.804 9.938 1.00 59.09 44.133 8.691 12.327 1.00 16.83

FIG. 7(49)

ATOM 2418 C GLU 1146 57.910 13.742 11.052 1.00 36.46 ATOM 2419 O GLU 1146 57.378 13.665 9.934 1.00 35.72 ATOM 2420 N PRO 1147 57.861 14.868 11.791 1.00 34.09 ATOM 2421 CD PRO 1147 58.490 15.147 13.099 1.00 33.72 ATOM 2422 CA PRO 1147 57.082 16.020 11.336 1.00 29.77 ATOM 2423 CB PRO 1147 57.446 17.106 12.351 1.00 27.86 57.668 16.334 13.619 1.00 26.72 ATOM 2424 CG PRO 1147 ATOM 2425 C PRO 1147 57.436 16.417 9.922 1.00 27.04 ATOM 2426 O PRO 1147 56.559 16.784 9.158 1.00 30.21 ATOM 2427 N SER 1148 58.698 16.255 9.551 1.00 22.56 59.177 16.616 8.210 1.00 24.23 ATOM 2429 CA SER 1148 ATOM 2430 CB SER 1148 60.707 16.724 8.203 1.00 27.40 ATOM 2431 OG SER 1148 61.314 15.477 8.545 1.00 36.19 ATOM 2433 C SER 1148 58.743 15.674 7.101 1.00 21.41 ATOM 2434 O SER 1148 58.890 15.964 5.913 1.00 24.41 58.272 14.508 7.485 1.00 25.45 ATOM 2435 N GLN 1149 57.831 13.547 6.497 1.00 26.28 58.224 12.142 6.946 1.00 32.79 59.705 11.907 6.958 1.00 25.96 ATOM 2437 CA GLN 1149 ATOM 2438 CB GLN 1149 59.705 11.907 6.958 1.00 25.96 ATOM 2439 CG GLN 1149 ATOM 2440 CD GLN 1149 60.279 12.196 5.622 1.00 32.77 59.765 11.744 4.591 1.00 36.63 ATOM 2441 OE1 GLN 1149 ATOM 2442 NE2 GLN 1149 61.312 13.007 5.604 1.00 37.86

 56.327
 13.670
 6.278
 1.00
 23.40

 55.783
 13.145
 5.306
 1.00
 23.12

 55.662
 14.339
 7.215
 1.00
 22.72

 ATOM 2445 C GLN 1149 ATOM 2446 O GLN 1149 ATOM 2447 N ARG 1150 54.226 14.22 53.721 15.243 8.392 1.00 13.96 54.161 14.532 9.598 1.00 13.96 53.285 14.903 10.728 1.00 15.08 ATOM 2449 CA ARG 1150 54.226 14.581 7.132 1.00 17.86 ATOM 2450 CB ARG 1150 ATOM 2451 CG ARG 1150 ATOM 2452 CD ARG 1150 53.285 14.903 10.728 1.00 15.08 ATOM 2453 NE ARG 1150 53.632 14.090 11.879 1.00 24.55 54.066 14.564 13.040 1.00 27.63 54.192 15.871 13.230 1.00 27.18 ATOM 2455 CZ ARG 1150 ATOM 2456 NH1 ARG 1150 54.423 13.717 13.991 1.00 29.34 ATOM 2459 NH2 ARG 1150 ATOM 2462 C ARG 1150 54.025 15.559 6.008 1.00 16.82 52.873 15.464 5.320 1.00 13.09 52.873 15.464 5.320 1.00 18.01 51.793 14.453 5.320 1.00 6.32 52.726 16.442 4.240 1.00 18.95 51.489 15.948 3.492 1.00 16.01 50.726 15.092 4 520 1.00 16.01 ATOM 2463 O ARG 1150 54.913 16.382 5.715 1.00 13.09 ATOM 2464 N PRO 1151 ATOM 2465 CD PRO 1151 ATOM 2466 CA PRO 1151 ATOM 2467 CB PRO 1151 ATOM 2468 CG PRO 1151

FIG. 7(50)

ATOM 2469 C PRO 1151 52.574 17.861 4.805 1.00 18.27 52.422 18.039 6.006 1.00 19.70 ATOM 2470 O PRO 1151 ATOM 2471 N THR 1152 52.763 18.860 3.958 1.00 19.16 ATOM 2473 CA THR 1152 52.604 20.251 4.366 1.00 14.92 ATOM 2474 CB THR 1152 53.511 21.138 3.560 1.00 13.80 ATOM 2475 OG1 THR 1152 53.146 21.080 2.163 1.00 17.02 ATOM 2477 CG2 THR 1152 54.918 20.697 3.764 1.00 5.40 51.196 20.571 3.979 1.00 13.16 ATOM 2478 C THR 1152 ATOM 2479 O THR 1152 50.682 19.905 3.084 1.00 19.18 ATOM 2480 N PHE 1153 50.561 21.572 4.599 1.00 14.62 ATOM 2482 CA PHE 1153 49.176 21.910 4.224 1.00 12.87 ATOM 2483 CB PHE 1153 48.588 23.023 5.083 1.00 11.95 ATOM 2484 CG PHE 1153 48.157 22.558 6.422 1.00 9.67 47.037 21.740 6.560 1.00 14.91 ATOM 2485 CD1 PHE 1153 ATOM 2486 CD2 PHE 1153 48.891 22.857 7.533 1.00 15.01 ATOM 2487 CE1 PHE 1153 46.660 21.215 7.802 1.00 9.44 ATOM 2488 CE2 PHE 1153 48.529 22.340 8.789 1.00 13.43 47.405 21.513 8.913 1.00 8.41 ATOM 2489 CZ PHE 1153 ATOM 2490 C PHE 1153 49.073 22.253 2.750 1.00 16.98 ATOM 2491 O PHE 1153 48.078 21.927 2.114 1.00 21.60 ATOM 2492 N SER 1154 50.116 22.841 2.168 1.00 15.39 50.031 23.123 0.754 1.00 17.55 ATOM 2494 CA SER 1154 ATOM 2495 CB SER 1154 51.251 23.868 0.254 1.00 25.28 51.244 25.190 0.776 1.00 33.35 ATOM 2496 OG SER 1154 ATOM 2498 C SER 1154 49.850 21.815 0.022 1.00 20.26 48.932 21.704 -0.798 1.00 23.74 ATOM 2499 O SER 1154 ATOM 2500 N GLU 1155 50.670 20.808 0.347 1.00 19.47 ATOM 2502 CA GLU 1155 50.534 19.493 -0.307 1.00 16.55 51.588 18.513 0.188 1.00 19.82 ATOM 2503 CB GLU 1155 ATOM 2504 CG GLU 1155 52.932 18.773 -0.486 1.00 20.20 ATOM 2505 CD GLU 1155 54.128 18.210 0.249 1.00 23.11 55.226 18.377 -0.312 1.00 35.76 ATOM 2506 OE1 GLU 1155 ATOM 2507 OE2 GLU 1155 54.009 17.631 1.359 1.00 21.09 ATOM 2508 C GLU 1155 49.153 18.918 -0.107 1.00 16.59 ATOM 2509 O GLU 1155 48.548 18.414 -1.055 1.00 21.37 48.619 19.034 1.101 1.00 16.01 ATOM 2510 N LEU 1156 47.272 18.532 1.375 1.00 18.06 ATOM 2512 CA LEU 1156 ATOM 2513 CB LEU 1156 . 46.969 18.521 2.875 1.00 15.74 ATOM 2514 CG LEU 1156 47.688 17.493 3.759 1.00 11.35 47.786 18.049 5.201 1.00 2.08 ATOM 2515 CD1 LEU 1156

FIG. 7(51)

ATOM 2516 CD2 LEU 1156 46.927 16.150 3.708 1.00 14.36 46.165 19.287 0.638 1.00 20.03 ATOM 2517 C LEU 1156 ATOM 2518 O LEU 1156 45.105 18.711 0.355 1.00 26.86 46.354 20.570 0.355 1.00 21.44 ATOM 2519 N VAL 1157 ATOM 2521 CA VAL 1157 45.303 21.283 -0.362 1.00 21.15 ATOM 2522 CB VAL 1157 45.513 22.801 -0.381 1.00 21.33 44.569 23.453 -1.368 1.00 15.98 ATOM 2523 CG1 VAL 1157 45.198 23.340 0.974 1.00 13.87 ATOM 2524 CG2 VAL 1157 ATOM 2525 C VAL 1157 45.270 20.721 -1.760 1.00 22.88 ATOM 2526 O VAL 1157 44.198 20.508 -2.333 1.00 25.54 46.445 20.400 -2.282 1.00 23.10 ATOM 2527 N GLU 1158 ATOM 2529 CA GLU 1158 46.503 19.815 -3.603 1.00 27.24 ATOM 2530 CB GLU 1158 47.922 19.756 -4.115 1.00 32.82 ATOM 2531 CG GLU 1158 47.969 18.978 -5.404 1.00 44.73 ATOM 2532 CD GLU 1158 49.187 19.268 -6.212 1.00 51.53 ATOM 2533 OE1 GLU 1158 49.007 19.887 -7.292 1.00 54.31 ATOM 2534 OE2 GLU 1158 50.298 18.869 -5.765 1.00 51.10 45.939 18.403 -3.643 1.00 26.42 ATOM 2535 C GLU 1158 ATOM 2536 O GLU 1158 45.167 18.051 -4.546 1.00 25.91 ATOM 2537 N HIS 1159 46.347 17.591 -2.669 1.00 26.36 ATOM 2539 CA HIS 1159 45,897 16.226 -2.611 1.00 21.52 ATOM 2540 CB HIS 1159 46.674 15.444 -1.576 1.00 25.28 ATOM 2541 CG HIS 1159 46.322 13.991 -1.545 1.00 24.66 46.408 13.030 -2.497 1.00 24.44 ATOM 2542 CD2 HIS 1159 ATOM 2543 ND1 HIS 1159 45.749 13.387 -0.452 1.00 21.30 ATOM 2545 CE1 HIS 1159 45.489 12.125 -0.731 1.00 23.16 45.879 11.884 -1.961 1.00 19.88 ATOM 2546 NE2 HIS 1159 ATOM 2548 C HIS 1159 44.402 16.104 -2.391 1.00 21.56 ATOM 2549 O HIS 1159 43.741 15.311 -3.066 1.00 22.19 ATOM 2550 N LEU 1160 43.852 16.874 -1.456 1.00 20.25 ATOM 2552 CA LEU 1160 42.408 16.832 -1.209 1.00 17.66 ATOM 2553 CB LEU 1160 42.111 17.502 0.130 1.00 17.84 42.676 16.760 1.352 1.00 20.17 ATOM 2554 CG LEU 1160 ATOM 2555 CD1 LEU 1160 42.472 17.542 2.619 1.00 21.45 ATOM 2556 CD2 LEU 1160 41.992 15.454 1.512 1.00 19.45 41.566 17.418 -2.395 1.00 17.71 ATOM 2557 C LEU 1160 40.426 17.030 -2.624 1.00 15.39 ATOM 2558 O LEU 1160 .ATOM 2559 N GLY 1161 42.130 18.356 -3.153 1.00 23.52 ATOM 2561 CA GLY 1161 41.434 18.879 -4.322 1.00 21.37 41.342 17.741 -5.346 1.00 23.91 ATOM 2562 C GLY 1161

FIG. 7(52)

ATOM 2563 O GLY 1161 40.295 17.526 -5.971 1.00 23.05 ATOM 2564 N ASN 1162 42.439 16.997 -5.520 1.00 21.49 ATOM 2566 CA ASN 1162 42.428 15.854 -6.428 1.00 22.31 ATOM 2567 CB ASN 1162 43.771 15.109 -6.427 1.00 22.34 ATOM 2568 CG ASN 1162 44.904 15.888 -7.062 1.00 20.03 ATOM 2569 OD1 ASN 1162 44.705 16.903 -7.701 1.00 28.17 46.117 15.401 -6.873 1.00 32.22 ATOM 2570 ND2 ASN 1162 ATOM 2573 C ASN 1162 41.356 14.851 -5.969 1.00 23.05 ATOM 2574 O ASN 1162 40.570 14.378 -6.769 1.00 26.11 ATOM 2575 N LEU 1163 41.360 14.490 -4.688 1.00 21.05 ATOM 2577 CA LEU 1163 40.405 13.523 -4.166 1.00 19.91 ATOM 2578 CB LEU 1163 40.695 13.172 -2.689 1.00 19.18 ATOM 2579 CG LEU 1163 41.675 12.042 -2.275 1.00 18.62 42.959 12.120 -3.020 1.00 24.35 ATOM 2580 CD1 LEU 1163 ATOM 2581 CD2 LEU 1163 41.983 12.043 -0.804 1.00 14.82 39.015 14.038 -4.331 1.00 19.71 ATOM 2582 C LEU 1163 ATOM 2583 O LEU 1163 38.110 13.318 -4.767 1.00 23.11 ATOM 2584 N LEU 1164 38.860 15.328 -4.121 1.00 25.91 ATOM 2586 CA LEU 1164 37.533 15.941 -4.226 1.00 29.28 ATOM 2587 CB LEU 1164 37.603 17.388 -3.726 1.00 31.25 ATOM 2588 CG LEU 1164 36.348 18.176 -3.371 1.00 25.75 ATOM 2589 CD1 LEU 1164 35.429 17.396 -2.435 1.00 31.52 ATOM 2590 CD2 LEU 1164 7.018 15.866 -5.653 1.00 30.07 ATOM 2592 O LEU 1164 35.953 15.330 -5.903 1.00 32.61 ATOM 2593 N GLN 1165 37.810 16.344 -6.598 1.00 33.76 ATOM 2595 CA GLN 1165 37.423 16.317 -8.003 1.00 39.95 ATOM 2596 CB GLN 1165 38.451 17.048 -8.855 1.00 46.90 ATOM 2597 CG GLN 1165 38.758 18.474 -8.480 1.00 49.81 ATOM 2598 CD GLN 1165 39.874 19.024 -9.348 1.00 56.23 ATOM 2599 OE1 GLN 1165 41.056 18.945 -8.997 1.00 55.97 ATOM 2600 NE2 GLN 1165 39.508 19.536 -10.518 1.00 60.66 37.304 14.898 -8.554 1.00 39.33 ATOM 2603 C GLN 1165 ATOM 2604 O GLN 1165 36.652 14.685 -9.568 1.00 42.09 ATOM 2605 N ALA 1166 38.059 13.965 -7.988 1.00 36.82 37.994 12.586 -8.441 1.00 34.66 ATOM 2607 CA ALA 1166 ATOM 2608 CB ALA 1166 39.096 11.748 -7.814 1.00 32.78 36.640 12.103 -7.991 1.00 36.63 ATOM 2609 C -ALA 1166 ATOM 2610 O ALA 1166 35.969 11.381 -8.713 1.00 39.47 36.226 12.532 -6.800 1.00 40.01 ATOM 2611 N ASN 1167 ATOM 2613 CA ASN 1167 34.911 12.158 -6.264 1.00 42.40

FIG. 7(53)

ATOM 2614 CB ASN 1167 34.641 12.878 -4.919 1.00 42.99 ATOM 2615 CG ASN 1167 33.354 12.409 -4.242 1.00 40.80 ATOM 2616 OD1 ASN 1167 32.306 13.046 -4.348 1.00 40.18 ATOM 2617 ND2 ASN 1167 33.436 11.294 -3.532 1.00 36.58 ATOM 2620 C ASN 1167 33.822 12.498 -7.299 1.00 41.88 ATOM 2621 O ASN 1167 32.837 11.789 -7.391 1.00 41.83 ATOM 2622 N ALA 1168 34.057 13.558 -8.085 1.00 45.09 ATOM 2624 CA ALA 1168 33.187 14.065 -9.160 1.00 46.02 ATOM 2625 CB ALA 1168 32.507 12.933 -9.929 1.00 45.92 ATOM 2626 C ALA 1168 32.181 15.123 -8.728 1.00 48.61 ATOM 2628 O ALA 1168 32,627 16,233 -8,363 1.00 50,20 ATOM 2629 O HOH 46.858 21.496 16.690 1.00 23.54 1 ATOM 2632 O HOH 2 49.904 21.605 17.271 1.00 36.65 **ATOM 2635 O HOH** 3 49.682 18.133 17.657 1.00 50.47 **ATOM 2638 O HOH** 4 56.606 19.394 15.202 1.00 25.28 ATOM 2641 O HOH 5 57.215 21.949 11.395 1.00 37.66 **ATOM 2644 O HOH** 6 56.082 25.850 12.933 1.00 34.63 7 52.355 23.016 6.377 1.00 21.45 ATOM 2647 O HOH **ATOM 2650 O HOH** 8 51.153 27.376 4.088 1.00 29.93 ATOM 2653 O HOH 9 44.820 28.454 1.120 1.00 16.47 **ATOM 2656 O HOH** 10 46.377 38.321 5.198 1.00 31.93 **ATOM 2659 O HOH** 11 43.987 38.133 3.129 1.00 52.41 ATOM 2662 O HOH 12 53.321 40.451 6.702 1.00 31.88 **ATOM 2665 O HOH** 13 44.977 49.530 8.305 1.00 44.56 **ATOM 2668 O HOH** 14 44.379 43.338 7.798 1.00 31.72 ATOM 2671 O HOH 39.477 40.232 8.468 1.00 36.65 15 **ATOM 2674 O HOH** 16 41.987 36.751 10.646 1.00 23.26 ATOM 2677 O HOH 17 41.711 41.873 6.802 1.00 34.79 **ATOM 2680 O HOH 18** 29.514 24.656 18.739 1.00 31.43 ATOM 2683 O HOH 19 27.493 22.351 15.517 1.00 42.03 **ATOM 2686 O HOH 20** 24.345 20.097 15.325 1.00 24.92 ATOM 2689 O HOH 21 32.381 18.452 20.520 1.00 75.12 **ATOM 2692 O HOH** 22 31.071 8.282 19.507 1.00 31.68 33.001 7.742 21.598 1.00 38.67 **ATOM 2695 O HOH** 23 34.802 6.439 18.667 1.00 34.24 **ATOM 2698 O HOH** 24 **ATOM 2701 O HOH** 25 32.273 6.932 14.174 1.00 41.21 **ATOM 2704 O HOH 26** 34.059 5.245 12.870 1.00 49.30 **ATOM 2707 O HOH 27** 3.432 4.799 1.00 63.69 38.059 28 **ATOM 2710 O HOH** 41.089 1.841 4.421 1.00 42.86 **ATOM 2713 O HOH** 29 45.081 9.234 -0.557 1.00 39.97

FIG. 7(54)

ATOM 2716 O HOH **30** 47.301 11.215 1.271 1.00 58.47 **ATOM 2719 O HOH** 31 50.046 14.055 0.168 1.00 37.58 ATOM 2722 O HOH **32** 54.425 8.937 4.821 1.00 36.74 52.279 7.099 5.152 1.00 13.04 **ATOM 2725 O HOH** 33 **ATOM 2728 O HOH** 34 53.025 7.510 7.740 1.00 25.53 **ATOM 2731 O HOH** 35 50.852 6.818 10.462 1.00 18.29 **ATOM 2734 O HOH** 46.448 7.762 15.254 1.00 9.08 **36 ATOM 2737 O HOH 37** 47.326 3.930 20.460 1.00 34.16 **ATOM 2740 O HOH** 38 48.264 12.367 20.804 1.00 22.14 **ATOM 2743 O HOH 39** 44.276 8.193 24.312 1.00 40.52 **ATOM 2746 O HOH** 40 37.491 11.237 25.975 1.00 38.71 **ATOM 2749 O HOH** 37.592 13.565 23.164 1.00 44.55 41 **ATOM 2752 O HOH** 42 34.887 12.418 26.235 1.00 50.96 **ATOM 2755 O HOH** 43 24.823 15.933 17.377 1.00 33.72 **ATOM 2758 O HOH** 44 23.302 7.532 7.049 1.00 57.56 **ATOM 2761 O HOH** 45 29.954 11.864 -3.109 1.00 38.05 **ATOM 2764 O HOH** 42.099 3.812 18.044 1.00 40.12 46 ATOM 2767 O HOH 47 38.653 0.737 18.003 1.00 37.30 **ATOM 2770 O HOH** 48 34.169 14.465 16.707 1.00 20.01 **ATOM 2773 O HOH** 49 37.055 32.622 16.570 1.00 31.20 **ATOM 2776 O HOH 50** 29.361 31.729 15.460 1.00 21.90 **ATOM 2779 O HOH** 51 25.866 31.495 10.192 1.00 24.50 **ATOM 2782 O HOH 52** 23.411 32.276 10.616 1.00 68.85 **ATOM 2785 O HOH** 53 22.135 37.404 8.648 1.00 40.22 **ATOM 2788 O HOH 54** 28.356 36.997 10.747 1.00 22.41 **ATOM 2791 O HOH 55** 29.650 33.190 8.897 1.00 31.98 **ATOM 2794 O HOH 56** 34.801 35.904 3.297 1.00 59.73 **ATOM 2797 O HOH** 57 24.341 20.715 4.934 1.00 28.10 **ATOM 2800 O HOH 58** 37.439 20.236 25.832 1.00 33.07 **ATOM 2803 O HOH 59** 32,675 51,977 19,122 1.00 33,52 **ATOM 2806 O HOH** 32.722 54.003 14.118 1.00 25.01 **60 ATOM 2809 O HOH** 61 29.691 54.769 22.004 1.00 27.32 **ATOM 2812 O HOH 62** 21.347 47.577 14.711 1.00 27.85 **ATOM 2815 O HOH 63** 25.640 44.257 7.516 1.00 24.71 24.686 40.916 3.785 1.00 55.13 **ATOM 2818 O HOH** 64 33.825 48.721 10.105 1.00 39.11 **ATOM 2821 O HOH** 65 **ATOM 2824 O HOH** 39.855 54.415 18.247 1.00 50.97 66 ATOM 2827 O .HOH 67 36.001 50.053 7.081 1.00 68.99 **ATOM 2830 O HOH 68** 37.973 50.651 5.331 1.00 32.12 40.220 53.227 6.506 1.00 15.02 **ATOM 2833 O HOH** 69

FIG. 7(55)

ATOM 2836 O HOH 70 42.258 51.833 6.993 1.00 21.05 ATOM 2839 O HOH 71 36.813 55.217 13.035 1.00 46.29 2842 O HOH 37.030 55.879 15.712 1.00 39.36 ATOM 72 ATOM 2845 O HOH 73 23.054 45.061 23.607 1.00 51.11 ATOM 2848 O HOH 74 27.075 54.516 6.971 1.00 51.66 ATOM 2851 O HOH **75** 21.634 54.039 13.651 1.00 36.36 45.158 47.529 30.699 1.00 56.11 ATOM 2854 O HOH 76 77 44.469 45.246 36.699 1.00 36.50 2857 O HOH ATOM ATOM 2860 O HOH **78** 45.882 41.717 36.085 1.00 28.57 ATOM 2863 O HOH **79** 49.406 41.527 34.292 1.00 65.94 ATOM 2866 O HOH 80 36.134 49.719 26.101 1.00 63.80 ATOM 2869 O HOH 26.884 28.564 16.554 1.00 49.20 81 ATOM 2872 O HOH 82 22.079 10.131 13.444 1.00 56.45 ATOM 2875 O HOH 41.225 4.655 30.464 1.00 58.98 83 ATOM 2878 O HOH 47.309 1.568 10.326 1.00 21.69 84 ATOM 2881 O HOH 56.613 18.335 6.527 1.00 33.97 85 ATOM 2884 O HOH 86 56.196 16.855 3.275 1.00 47.24 ATOM 2887 O HOH 87 54.826 22.813 0.598 1.00 33.50 ATOM 2890 O HOH 52.962 21.915 -2.351 1.00 66.62 88 47.896 24.242 -3.714 1.00 40.99 ATOM 2893 O HOH 89 ATOM 2896 O HOH 90 40.295 22.360 25.551 1.00 39.81 ATOM 2899 O HOH 40.188 3.202 15.661 1.00 45.97 91 ATOM 2902 O HOH 92 45.159 2.965 19.553 1.00 44.25 ATOM 2905 O HOH 36.591 7.772 23.374 1.00 68.23 93 34.274 5.197 22.878 1.00 51.62 ATOM 2908 O HOH 94 ATOM 2911 O HOH 95 41.935 7.033 29.073 1.00 63.23 ATOM 2914 O HOH 20.731 12.105 14.716 1.00 54.80 96 ATOM 2917 O HOH 23.147 13.682 17.882 1.00 50.81 97 ATOM 2920 O HOH 98 35.515 9.509 -3.558 1.00 56.70 ATOM 2923 O HOH 99 38.933 9.503 -1.231 1.00 32.18 ATOM 2926 O HOH 100 51.814 24.438 3.703 1.00 52.00 ATOM 2929 O HOH 101 51.670 28.690 0.838 1.00 42.41 ATOM 2932 O HOH 102 46.536 30.610 1.750 1.00 45.80 ATOM 2935 O HOH 103 45.165 34.214 0.818 1.00 46.46 ATOM 2938 O HOH 104 42.695 35.194 1.055 1.00 25.82 ATOM 2941 O HOH 105 39.689 33.418 0.723 1.00 31.99 MOTA 2944 O HOH 106 23.962 38.119 27.549 1.00 47.89 25.343 40.908 27.379 1.00 54.09 MOTA 2947 O HOH 107 2950 O **HOH 108** 20.307 35.738 19.866 1.00 32.61 MOTA ATOM 2953 O HOH 109 28.085 54.303 18.810 1.00 61.58

FIG. 7(56)

ATOM 2956 O HOH 110 29.849 56.131 16.966 1.00 37.29 ATOM 2959 O HOH 111 31.503 58.023 14.735 1.00 46.45 ATOM 2962 O HOH 112 35.212 55.981 10.499 1.00 92.07 ATOM 2965 O HOH 113 36.530 55.812 6.656 1.00 30.72 ATOM 2968 O HOH 114 50.045 41.251 26.059 1.00 82.26 ATOM 2971 O HOH 115 25.153 36.460 9.054 1.00 50.86 31.749 32.705 15.359 1.00 30.04 ATOM 2974 O HOH 116 ATOM 2977 O HOH 117 30.213 3.806 4.940 1.00 39.74 ATOM 2980 O HOH 118 36.511 1.159 7.275 1.00 41.62 ATOM 2983 O HOH 119 27.155 4.637 5.224 1.00 79.92 ATOM 2986 O HOH 120 57.319 11.287 3.459 1.00 33.02 ATOM 2989 O HOH 121 52.121 12.483 1.755 1.00 45.55 ATOM 2992 O HOH 47.613 14.088 -5.021 1.00 41.01 122 ATOM 2995 O HOH 123 57.550 26.628 16.551 1.00 30.62 MOTA 2998 O HOH 124 32.338 10.125 23.559 1.00 35.48 31.065 5.698 3.273 1.00 42.74 3001 O HOH 125 MOTA ATOM 3004 O HOH 126 32.603 4.523 1.410 1.00 33.30 ATOM 3007 O HOH 127 34.394 2.617 4.702 1.00 42.12 ATOM 3010 O HOH 128 37.961 10.373 -4.287 1.00 47.57 MOTA 3013 O HOH 129 42.215 11.947 -6.970 1.00 45.13 ATOM 3016 O HOH 130 46.307 8.952 -4.280 1.00 70.02 3019 O HOH 131 MOTA 50.369 17.388 -3.277 1.00 42.22 MOTA 3022 O HOH 132 47.231 21.866 22.930 1.00 50.84 ATOM 3025 O HOH 133 45.362 17.669 27.147 1.00 48.06 ATOM 3028 O HOH 134 27.005 23.141 18.124 1.00 49.65 ATOM 3031 O HOH 135 45.726 12.511 -6.453 1.00 45.31 MOTA 3034 O HOH 136 46.998 11.755 18.088 1.00 37.38 ATOM 3037 O HOH 137 39.706 37.699 9.894 1.00 40.71 MOTA 3040 O HOH 138 18.768 48.678 17.798 1.00 74.62 MOTA 3043 O HOH 139 43.641 47.080 26.762 1.00 44.64 3046 O HOH 140 MOTA 32.593 53.980 16.744 1.00 43.95 MOTA 3049 O HOH 141 34.726 55.568 14.399 1.00 45.86 ATOM 3052 O HOH 142 30.551 53.227 19.638 1.00 35.99 MOTA 3055 O HOH 143 26.370 55.161 14.300 1.00 33.09 3058 O HOH 144 MOTA 24.547 55.803 6.815 1.00 58.70 3061 O HOH 145 36.217 52.574 3.221 1.00 68.48 MOTA 3064 O HOH 146 39.065 54.455 4.595 1.00 48.85 MOTA MOTA 3067 O HOH 147 45.130 40.725 5.433 1.00 62.58 MOTA 3070 O HOH 148 33.453 43.988 7.386 1.00 41.59 ATOM 3073 O HOH 149 36.626 45.045 6.144 1.00 54.04

FIG. 7(57)

ATOM 3076 O HOH 150 19.458 36.977 14.386 1.00 56.50 ATOM 3079 O HOH 151 19.502 40.993 17.850 1.00 43.35 ATOM 3082 O HOH 152 39.793 38.257 27.760 1.00 63.31 ATOM 3085 O HOH 153 40.730 53.944 20.682 1.00 49.91 ATOM 3088 O 45.371 49.402 5.710 1.00 41.53 HOH 154 ATOM 3091 O HOH 155 49.114 26.038 11.482 1.00 34.43 ATOM 3094 O HOH 156 54.085 28.403 10.828 1.00 28.60 ATOM 3097 O HOH157 18.729 14.990 12.752 1.00 44.66 ATOM 3100 O HOH 27.500 2.046 10.138 1.00 47.88 158 ATOM 3103 O HOH 159 23.505 7.763 16.082 1.00 45.49 ATOM 3106 O HOH 160 38.101 22.326 23.406 1.00 43.42 ATOM 3109 O HOH 161 36.788 33.961 0.261 1.00 59.95 ATOM 3112 O HOH 162 19.380 27.777 6.595 1.00 56.29 ATOM 3115 O HOH 33.583 33.343 17.339 1.00 68.25 163 ATOM 3118 O HOH 164 43.221 53.467 17.853 1.00 62.89 ATOM 3121 O HOH 165 28.154 41.110 29.042 1.00 61.19 ATOM 3124 O HOH 44.877 47.914 12.583 1.00 21.27 166 ATOM 3127 O HOH 167 46.589 45.908 14.329 1.00 39.48 ATOM 3130 O 48.235 43.490 14.297 1.00 46.88 HOH 168 ATOM 3133 O HOH 47.834 0.528 14.762 1.00 74.55 169 ATOM 3136 O HOH 170 48.711 -2.009 16.386 1.00 52.45 ATOM 3139 O HOH 41.210 0.396 17.381 1.00 58.05 171 ATOM 3142 O HOH 172 43.837 1.538 17.483 1.00 72.30 ATOM 3145 O HOH 173 41.780 -2.478 14.396 1.00 47.15 ATOM 3148 O HOH 174 31.466 11.699 21.418 1.00 45.99 ATOM 3151 O HOH 175 35.046 14.218 20.429 1.00 39.37 ATOM 3154 O HOH 176 22.639 26.143 4.324 1.00 36.80 3157 O HOH 177 26.114 24.452 6.028 1.00 31.04 MOTA 28.927 30.687 4.252 1.00 41.38 ATOM 3160 O HOH 178 3163 O HOH 179 MOTA 23.899 6.610 18.621 1.00 56.43 ATOM 3166 O HOH 180 53.386 11.969 4.493 1.00 39.86 HOH 181 ATOM 3169 O 30.051 43.727 0.910 1.00 47.97 ATOM 3172 O HOH 182 31.659 49.099 8.149 1.00 52.84